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ORIGINAL

Risk Assessment Methodology Development for Waste Isolation in Geologic Media

Technical Review of Documents NUREG/CR-1262, NUREG/CR-1376, NUREG/CR-1377, NUREG/CR-1397, and NUREG/CR-1608

Prepared by C. A. Stevens, R. R. Fullwood, S. L. Basin

Science Applications, Inc.

Prepared for
U.S. Nuclear Regulatory
Commission

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ABSTRACT

A review of five documents that were prepared for the USNRC by Sandia Laboratories is presented in this report. The documents covered in the present review include: NUREG/CR-1262, NUREG/CR-1376, NUREG/CR-1377, NUREG/CR-1397 and NUREG/CR-1608. This constitutes the second phase of the review; the first phase was reported in Volume 1 of NUREG/CR-1672, November 1980. Two of the documents concern simplified computational methods illustrative of the calculations necessary to produce a response surface. Three of the reports pertain to statistical methods, including the application of Latin hypercube Sampling (LHS).

The following observations have been made relative to the above reports: (1) the reports are, in general, difficult to read, due, in part, to unnecessarily complicated notation and lack of adequate explanation and examples, (2) the relationship of the work to similar work in the U.S. and abroad is not discussed, and (3) limitations of the LHS method are not discussed in sufficient depth.

The Sandia's response to this review is published as NUREG/CR 2428. Volume 1 is scheduled for completion in June 1982.

1.0 SUMMARY

The review procedure used for the five documents in Phase II was similar to that of Phase I. Specifically, a sub-committee of five individuals, each a specialist in one or more aspects of geological nuclear waste risk analysis, reviewed all five documents and provided comments. The review was conducted on three levels. The first level could be termed scientific and the procedures were similar to those used by the Lewis Committee in the review of WASH-1400. The second level attempted to discern the direction of licensing of geological nuclear waste repositories from the proposed 10CFR60, and to relate it to the documents being reviewed. From this, the following criteria, which are of use in assessing the applicability of the Sandia work to the licensing of a repository emerge: no canister leakage for the first 1,000 years and, after that, the leak rate of any isotope must be at most one part in 100,000 of the maximum amount of that radionuclide calculated to be present in the underground facility at any time after 1,000 years following permanent closure. The third level of the review was based on contract specified criteria, namely a list of questions prepared by the NRC. These criteria were not directly applicable to all the documents.

The first report (NUREG/CR-1262) introduces a method for inducing rank correlation among the input variables. The method is supposed to be distribution-free. In general, the report is difficult to understand. Limitations of the method are not discussed. The numerical examples are somewhat abstract, and do not illustrate the value of the procedure relative to Latin hypercube sampling (LHS). In addition, there is no discussion relative to why rank correlation was chosen over other alternatives. Intuitively, it seems as though the task of hypothesizing various degrees of rank correlation would be difficult.

The second report (NUREG/CR-1376) describes a simplified one-dimensional method called the Distributed Velocity Method (DVM) for calculating radionuclide transport. It is based upon the idea that the flow from a donor point to a receptor point results in a distributed velocity as a result of diffusion. This point-to-point response is related to a Green's function solution which is applied to the one-dimensional transport equation. This is extended to include radionuclide chains. Results from the DVM are compared with SWIFT, GETOUT, the method of characteristics and an analytic solution. DVM appears to be useful when performing sensitivity analyses and the calculation of repository release rates for simple repository geometries. The report would benefit from a discussion of the relationship between DVM and similar codes already in existence.

The third report (NUREG/CR-1377) presents a comparison between the one-dimensional Network Flow and Transport (NWFT) code for calculating repository release rates and the SWIFT code. Three scenarios are considered: (1) U-tube with river discharge, (2) U-tube with well discharge, and (3) hydraulic connection between overlying and underlying aquifers. The results are expressed in terms of the cumulative discharge. The effects of the independent variables or parameters are expressed in terms of standardized regression coefficients. For solubility limited scenarios, the important variables appear to be the solubility limit and the distribution coefficient; for leach limited cases, the important variables appear to be the leach time and the distribution coefficient. The generality of these conclusions is not fully explored.

A generalization of the Latin hypercube sampling method is presented in the fourth report (NUREG/CR-1397). This document contains comparisons of sampling methods and sample sizes. The methods are illustrated by applying them to a bedded salt repository with a U-tube hydraulic connection between the repository and an overlying aquifer. The report is relatively difficult to read due, in part, to overly complicated notation and the lack of adequate examples. However, this report illustrates, better than the other reports, how LHS is to be used as a practical analysis tool.

Report 5 (NUREG/CR-1608) describes a model called the deterministic-probabilistic contaminant transport (DPCT) model. This model provides a method for performing two-dimensional analyses of disrupted repositories. DPCT uses the groundwater flow field as the dominant component of radionuclide migration. This is the deterministic part which is obtained via SWIFT calculations. A random component is introduced via the use of a Gaussian distribution whose variance is related to the dispersion coefficient. DPCT is applied to 25 cases, 19 of which involve a bedded salt repository. Six cases involve a repository in fractured granite. The model is verified by comparing its results with those obtained by a one-dimensional analytic solution. The model, in its present form, does not treat radioactive decay chains. The data used in the calculations are rather conservative and there is some question as to the accuracy of representing ion-exchange retardation.

Overall, it is not clear how the reports support the objective of providing a risk methodology suitable for the licensing of repositories. Also, it is not exactly clear how the five reports, or the methodologies contained in the five reports, are related. For example, there are four codes for calculating radionuclide transport that have been developed as part of this program. The specific purpose of each of these is not explained. The requirement for monotonicity (a sufficient condition) for use of the LHS method may be a constraint that abrogates the advantages of LHS.

The Sandia's response to this review is published as NUREG/CR 2428. Volume 1 is scheduled for completion in June 1982.

2.0 INTRODUCTION

2.1 Background

Science Applications, Inc. (SAI), has been requested, by the Nuclear Regulatory Commission (NRC), to provide an independent multidisciplinary review and critique of technical reports which constitute the products of a project entitled "Risk Assessment Methodology Development for Waste Isolation in Geologic Media". These reports have been prepared by Sandia Laboratories for the Commission. The first phase of the project consisted of a review of the first three reports produced by Sandia. These reports were:

1. NUREG/CR-0458 (SAND78-0029), Risk Methodology for Geologic Disposal of Radioactive Waste: Interim Report, by J. E. Campbell, et. al., October 1978,
2. NUREG/CR-0394 (SAND78-0912), Risk Methodology for Geologic Disposal of Radioactive Waste: Sensitivity Analysis Techniques, by R. L. Iman, J. C. Helton, and J. E. Campbell, October 1978,
3. NUREG/CR-0424 (SAND78-1267), Risk Methodology for Geologic Disposal of Radioactive Waste: The Sandia Waste Isolation Flow and Transport (SWIFT) Model, by R. T. Dillon, R. B. Lantz, and S. B. Pahwa, October 1978, and associated computer code and user's manual describing SWIFT.

The results of the first phase were reported in Volume I of NUREG/CR-1672. In the second phase, SAI was requested to review the following documents:

1. NUREG/CR-1262 (SAND80-0157), Risk Methodology for Geologic Disposal of Radioactive Waste: A Distribution Free Approach to Inducing Rank Correlation Among Input Variables for Simulation Studies, by Ronald L. Iman and W. J. Conover, March 1980,
2. NUREG/CR-1376 (SAND80-0717), The Distributed Velocity Method of Solving the Convective Dispersion Equation, by James E. Campbell, Dennis E. Longsine, and Mark Reeves, July 1980,

3. NUREG/CR-1377 (SAND80-0644), Risk Methodology for Geologic Disposal of Radioactive Waste: Transport Model Sensitivity Analysis,, by James E. Campbell, Ronald L. Iman, and Mark Reeves, June 1980,

4. NUREG/CR-1397 (SAND80-0020), Risk Methodology for Geologic Disposal of Radioactive Waste: Small Sample Sensitivity Analysis Techniques for Computer Models, With An Application to Risk Assessment, by Ronald L. Iman, W. J. Conover, and James E. Campbell, March 1980,

5. NUREG/CR-1608 (CGS/NR85F060), Scenario Development and Evaluation Related to the Risk Assessment of High Level Radioactive Waste Repositories, by F. W. Schwartz and F. A. Donath, June 1980.

The fifth report represents work done by CGS, Inc., while the others report the work carried out by Sandia Laboratories. In addition to these documents, the reviewers were supplied with several supporting documents which served as background and reference material. The supporting documents include:

1. NUREG/CR-1190 (SAND79-1920), Risk Methodology for Geologic Disposal of Radioactive Waste: The Network Flow and Transport (NWFT) Model, by James E. Campbell, et. al., February 1980.

2. SAND79-1472, Stepwise Regression with PRESS and Rank Regression (Program User's Guide), by Ronald L. Iman, et. al., January 1980.

3. SAND79-1473, Latin Hypercube Sampling (Program User's Guide), by Ronald L. Iman, James M. Davenport, and Diane K. Zeigler, January 1980.

4. NUREG/CR-1609 (CGS/NR85F060), A Deterministic-Probabilistic Model for Contaminant Transport User's Manual, by F. W. Schwartz and A. Crowe, May 1980.

The review of each report was to be approached from the perspective of how well the report stands on its own as well as how it supports the overall Risk Methodology for Waste Isolation project.

During phase I, SAI assembled a panel of experts whose collective knowledge spans all of the technical areas covered in the reports reviewed during that phase and the areas expected to be covered in later phases of this project. In-depth reviews were performed by a sub-panel selected on the basis of technical expertise, availability and absence of conflict of interest. A similar sub-panel, whose members had served in that capacity during the first phase, was selected for phase II. Its members consisted of: B. Amirijafari, S. Basin, R. Fullwood, D. Ross-Brown, and C. Stevens.

The management and coordination for the review effort was performed by a technical coordinator and a management coordinator. The technical coordinator, Dr. R. Fullwood, had the responsibility for the technical content of this final report. The management coordinator, Dr. C. Stevens, had the responsibility for the technical editing of the final report and for the overall project management.

In order to assure that the review be independent, several restrictions were imposed on the sub-panel. Basically, these were:

1. No contact was to be made between the SAI reviewers and the Sandia personnel engaged in the study.
2. Essentially, no guidance was to be given by the NRC on how the review was to be conducted, other than that supplied in writing in the Contract Work Statement.
3. The SAI reviewers were not to be involved in other programs for the Department of Energy or otherwise be involved in projects which would lead to an actual or perceived conflict of interest.

All of these restrictions were complied with during the review period. Although there was no restriction on the use of outside consultants to assist in the review, none were used for the reports reviewed during phase II.

2.2 Report Arrangement

This report has been arranged to provide increasing depth of treatment as the reader progresses through it. An executive may obtain a capsule summary from the abstract and a bit more depth from the Summary. A specialist may be concerned with the organization, objectivity and independence of the review team such as has been presented in Section 1. Section 2 addresses the basis for the review. This is presented in three levels. The reviewers also worked with certain contract-specified general criteria in mind. The first level was the Lewis Committee criticisms of WASH-1400, a report that is not directly applicable to assessing the risk of a nuclear waste repository. Nevertheless, it was felt that there is some applicability of the Lewis Committee comments to the work at hand. The second level of the review was provided by the March 5, 1981 draft of 10CFR60. It may be deemed unfair to apply recent Federal regulations to previously prepared documents, however, it is likely that the methods being developed will have to be applied within this framework. The contract-specified criteria represent the last level.

The results of the review are presented in Section 3. Section 3.1 provides an overview of the set of five reports and attempts to view the interrelationships of the reports; Section 3.2 contains a general critique of each of the reports from the viewpoint that each report is supposed to be more or less self-contained and capable of being understood without extensive reference to other material. This is followed by references and five appendices, one for each report. Each appendix contains line-by-line comments presented by the reviewers. It was felt that by providing these reviews at these various levels, the utmost in objectivity could be achieved with good substantiation for the comments. In many cases, it was felt that the information contained in the reports was poorly presented; however, the reviewers attempted to ascertain the intent of the authors and the underlying verities.

2.3 Review Procedure

The review procedure was similar to that described in Section 1.3 of NUREG/CR-1672 (Vol. I), with one exception. Instead of distributing the reports to all of the panel members for an initial rapid reading, the reports were distributed only to members who were selected to perform in-depth reviews. These members, all of whom had served on the sub-panel for the phase 1 reviews, were selected on the basis of their technical specialty and how it relates to the specific documents to be reviewed in phase 2. Availability was another important consideration.

All members were encouraged to avoid being critical when it served no constructive purpose. When important points were found, the reviewers were encouraged to suggest improvements, compare with other authors or to note unresolved weaknesses common to many analyses.

The measures used by the reviewers may be as revealing as the results of the review itself. It may be said that three levels of review were in the minds of the reviewers. The first level derives from the Lewis Committee review of WASH-1400 (NUREG/CR-0400). The nature of this review may be described by the following attributes: completeness, auditability and scientific integrity. In the second level, the reviewers attempted to anticipate future licensing trends in order to judge the applicability of the methodology to future licensing requirements. The third level of the review consisted of the set of 9 criteria specified in the contract work statement.

2.4 Inferences from the Lewis Committee Review of WASH-1400

The Reactor Safety Study (RSS-WASH-1400) (1) was issued in draft form and was widely reviewed and issued about one year later in final form. Appendix XI of the RSS presents the criticisms of the draft report, some of which were addressed in the final report and some of which were applicable to the final report. Only a few critiques of the final report have been published (2,3). Of these, the Lewis Committee's criticisms (3) are the most recent. They draw on past critiques and are the most constructive and balanced. No attempt is made here to summarize the contents of the Lewis Committee report; however, several major points might be enlightening and relevant to the present review.

The major findings of the Lewis Committee were:

1. "Despite its shortcomings, WASH-1400 provides at this time the most complete single picture of accident probabilities associated with nuclear reactors. The fault tree/event tree approach coupled with an adequate data base is the best available tool with which to quantify these probabilities.

2. "We are unable to determine whether the absolute probabilities of accident sequences in WASH-1400 are high or low, but we believe that the error bounds on those estimates are, in general, greatly understated. This is true in part because there is in many cases an inadequate data base, in part because of an inability to quantify common cause failures, and in part because of some questionable methodological and statistical procedures.

3. "It should be noted that the dispersion model for radioactive material developed in WASH-1400 for reactor sites as a class cannot be applied to individual sites without significant refinement and sensitivity tests.

4. "The biological effects models should be updated and improved in the light of new information.

5. "After having studied the peer comments about some important classes of initiating events, we are unconvinced of the correctness of the WASH-1400 conclusion that they contribute negligibly to the overall risk. Examples include fires, earthquakes, and human accident initiation.

6. "It is conceptually impossible to be complete in a mathematical sense in the construction of event trees and fault trees; what matters is the approach to completeness and the ability to demonstrate with reasonable assurance that only small contributions are omitted. This inherent limitation means that any calculation using this methodology is always subject to revision and to doubt as to its completeness.

7. "The statistical analysis in WASH-1400 leaves much to be desired. It suffers from a spectrum of problems, ranging from lack of data on which to base input distributions to the invention and use of wrong statistical methods. Even when the analysis is done correctly, it is often presented in so murky a way as to be very hard to decipher.

8. "For a report of this magnitude, confidence in the correctness of the results can only come from a systematic and deep peer review process. The peer review process of WASH-1400 was defective in many ways and the review was inadequate.

9. "Lack of scrutability is a major failing of the report, impairing both its usefulness and the quality of possible peer review."

Item 1 is taken to be an endorsement of risk analysis itself. Fault trees and event trees were used in the RSS; Campbell et. al. (4) rejected this methodology for a hybrid approach that includes a combination of probabilistic as well as deterministic models. It is important to note that none of the reports reviewed deal with the probability of disruptive events; they are assumed to occur.

We must agree that absolute probabilities are less reliable than the ratios of predicted probabilities. The Sandia work has placed great emphasis on statistical procedures for sensitivity studies.

Item 3 is not directly applicable to the present review; however, it should be pointed out that aquatic dispersion is perhaps less understood or developed than meteorological dispersion.

Biological effects of radiation are continually being revised (item 4). The new BEIR reports may result in further revision. The reports reviewed in this phase do not treat human uptake or health effects.

Campbell et. al. (4) presented a discussion of disruptive events (item 5). How complete the treatment of a specific site is, remains to be seen.

The treatment presented in the five documents lacks completeness. Specifically, only disruptive events are considered. There is no investigation of an initiating event that does not result in a release because of some mitigating event. It may be claimed that exploring the set of events that do not impact man is a very extensive task; however, this is a part of completeness. Ignoring this part of the problem could result in misleading probability estimates. It also seems inconsistent to assume that geological changes initiate the disruption and at the same time treat the geology as static in the nuclide migration calculation.

As far as item 7 in the above list is concerned, the statistical aspects of the Sandia documents suffers from some of the same problems.

Item 8, regarding the auditability, is a serious defect of the Sandia work. If plausibility arguments could be presented using simple examples, confidence in the results would be strengthened. The relevance of natural occurrences such as the Oklo event to the methodology developed in the reports would also strengthen confidence in the results.

The documents lack scrutability (item 9). In may cases, this is because of poor presentation and lack of adequate examples. It is certainly not because the ideas are too complex to grasp.

2.5 Applicability to Licensing

The basis of this section is the proposed rule - 10CFR60, "Disposal of High-Level Radioactive Wastes in Geological Repositories: Technical Criteria," dated March 5, 1981. No attempt will be made to summarize this lengthy rule but excerpts will be taken as they relate to the review of the Sandia work.

Proposed 10CFR60 says that three barriers will be considered: (1) waste form and packaging, (2) underground facility, and (3) the site. The waste form and packaging are to be designed to confine the wastes for 1000 years after emplacement. These packages are to be retrievable within the first 50 years after emplacement.

The geologic setting of the site must exhibit structural and tectonic stability since the start of the Quaternary Period. It must also exhibit, over this period, hydrogeologic, geochemical and geomorphic stability. The repository must be located so that the pre-waste emplacement ground water travel times through the far field to the accessible environment are at least 1,000 years. The site should have a low population density and the mineral resources should have no more value than the average in the surrounding area.

The disturbed zone which is assumed to be its actual size or 2 km horizontally from the limits of the underground facility and from the surface to a depth of 500 meters below the limits of the excavation should be free of the following properties:

(i) Evidence of mining for resources unless it is entirely within the accessible environment.

(ii) Evidence of drilling for whatever purpose unless it is entirely within the accessible environment.

(iii) Resources that are economically exploitable using existing technology under present market conditions.

(iv) Resources that have either greater gross value, net value, or commercial potential than the average for other representative areas of similar size that are representative of and located in the geologic setting.

(v) Resources that have greater commercial potential based on a resource description, than the same resources in other areas that are representative of and located in the geologic setting.

(vi) Evidence of extreme erosion during the Quaternary Period.

(vii) Evidence of dissolutioning of soluble rocks.

(viii) The existence of a fault that has been active during the Quaternary Period.

(ix) Potential for creating new pathways for radionuclide migration due to presence of a fault or fracture zone irrespective of the age of last movement.

(x) Structural deformation such as uplift, subsidence, folding, and fracturing during the Quaternary Period.

(xi) More frequent occurrence of earthquakes or earthquakes of higher magnitude than is typical of the geologic setting.

(xii) Indications, based on correlations of earthquakes with tectonic processes and features, that either the frequency of occurrence or magnitude of earthquakes may increase.

(xiii) Evidence of igneous activity since the start of the Quaternary Period.

(xiv) Potential for changes in hydrologic conditions that would affect the migration of radionuclides to the accessible environment including but not limited to hydraulic gradient, average interstitial velocity, storage coefficient, hydraulic conductivity, natural recharge, potentiometric levels, and discharge points.

(xv) Conditions in the host rock that are not reducing conditions.

(xvi) Groundwater conditions in the host rock, such as high ionic strength or ranges of Eh-pH, that would affect the solubility and chemical reactivity of the engineered systems.

(xvii) Processes that would reduce sorption, result in degradation of the rock strength, or adversely affect the performance of the engineered system.

(xviii) Rock or groundwater conditions that would require complex engineering measures in the design and construction of the underground facility or in the sealing of boreholes and shafts.

(xix) Geomechanical properties that do not provide stability of underground openings during construction, and waste emplacement and retrieval operations.

This list provides some of the siting requirements. In addition, realistic analyses using conservative assumptions should be performed to determine the degree to which each of the favorable and adverse conditions, if present, has been characterized and the extent to which it contributes to isolation. Representative and bounding values shall be determined appropriate to the degree of resolution used in the analysis. These analyses and models used to predict future conditions and changes in the geologic setting shall be validated using field tests, on-site tests, field-verified laboratory tests, monitoring data, or natural analog studies.

These requirements also state that shaft and borehole seals shall not be in a preferential water pathway. These shaft and borehole seals must accommodate potential variations of stress, temperature and moisture. The seals should consist of multicomponents and use material compatible with the geochemistry of the rock, groundwater and anticipated rock deformation.

This completes our summary of the proposed 10CFR60. Relative to the present work, it defines zero leakage from the waste packages for the first 1,000 years and thereafter defines that the annual release of any radionuclide shall not exceed 1 part in 10^5 of the amount present in the repository. The proposed regulation does not require a risk analysis; it requires a leakage analysis subject to unspecified events over an unspecified time. In this regard, the reports reviewed are appropriate to the leakage analysis; however, the extensive error and sensitivity analysis seems to lose meaning unless some confidence bounds are to be placed on the 10^{-5} leak rate.

The other change which could result from the proposed 10CFR60 is the equal footing between waste form and packaging, repository and siting. Until recently, the U. S. approach was to place primary reliance on the geological barriers. The Sandia work is consistent with this previous approach.

2.6 Contract-Specified Review Criteria

The criteria, presented in the form of questions, are very similar to those used in Volume 1 of NUREG/CR-1672. It should be stated that it is difficult to devise criteria that will apply equally to the five different documents. In some cases, the criteria did not fit the documents at all. The contract specified criteria are stated in the form of a series of questions which are as follows:

1. Are the models realistic?
    a. Are the assumptions valid?
    b. What would be the impact on the analysis results of any incorrect assumptions?
    c. How should any identified weaknesses in the models be improved?
2. Is the methodology valid?
3. Are the data valid?
    a. What uncertainty in the data would render the model results unrealistic?
    b. Was each datum uncertainty and its contribution to the uncertainty in the results assessed appropriately?
4. Do the event sequences chosen for calculation cover a reasonably complete range?
    a. Is the treatment of completeness by Sandia and CGS adequate?
    b. Were any important potential risk contributors omitted? If so, identify.
    c. Were the quantitative or qualitative criteria for choice of sequencs valid?
    d. What were the criteria used as a basis for the selection of sequences for detailed examination and calculation by Sandia and CGS?

    e. Was a comparison made between the scenarios examined by Sandia and those examined by CGS? What were the differences and inconsistencies? How should these be resolved?

5. Was an effort made to identify (i.e., rank according to importance) the risk, key parameters, processes and events?

    a. If so, was the effort adequate?

    b. Evaluate the methods used to achieve the ranking.

6. Were the uncertainties in the results considered?

    a. Were these uncertainties propagated and quantified?

    b. Were acceptable numerical methods used?

    c. Were the contributing uncertainties correctly assessed?

7. Which of the models and which parts of the methodology could be used to resolve discrete questions (e.g., for a licensing review) or would they only be useful as supporting information to discrete questions?

    a. What types of questions could be resolved by use of a given model or the methodology?

8. Is there a correlation on scenario development between Sandia and CGS? What are the criteria in selecting the scenarios by both parties?

Each of the above questions will be considered in the detailed review which follows.

[redacted]

3.0 REVIEW AND CRITIQUE OF THE DOCUMENTS

3.1 Overview of the Set

Figure 3-1 presents the taxonomy of the risk methodology reports that have been reviewed to date. The report by Campbell et. al. (4) provides a general outline of the project. It contains a discussion of the disruptive event initiators and describes a deterministic-probabilistic methodology for estimating the likelihood of the repository disruption. It also describes a method of predicting nuclide transport rates (SWIFT), presents a compartment model for describing the pathways to man. The report ends with a discussion of dosimetry. The other reports in both Phase I and Phase II deal with simplified nuclide transport calculations and statistical methods involving sensitivity analysis and/or response surface modeling. The work reviewed in the present phase focuses on sensitivity analysis and nuclide migration calculations. The statistical topics all have to do with sampling; the applications aspect involves various computationally efficient ways to predict nuclide migration.

Although it is agreed that an uncertainty analysis is highly desirable if not the sine qua non of any quantitative risk estimate, there are many other aspects of risk assessment. A general outline is provided in Campbell et. al.(4). This consists of four basic steps: probability of disruption, nuclide migration, biosphere transport, and health effects. It seems that only the second of these, and in a sense, a subset of that one is being pursued. Besides these four major topics, support activities such as data base construction, selection of appropriate statistical distributions, scenario evaluations, etc., are apparently not being done. Thus, the reviewers question the emphasis placed in the work.

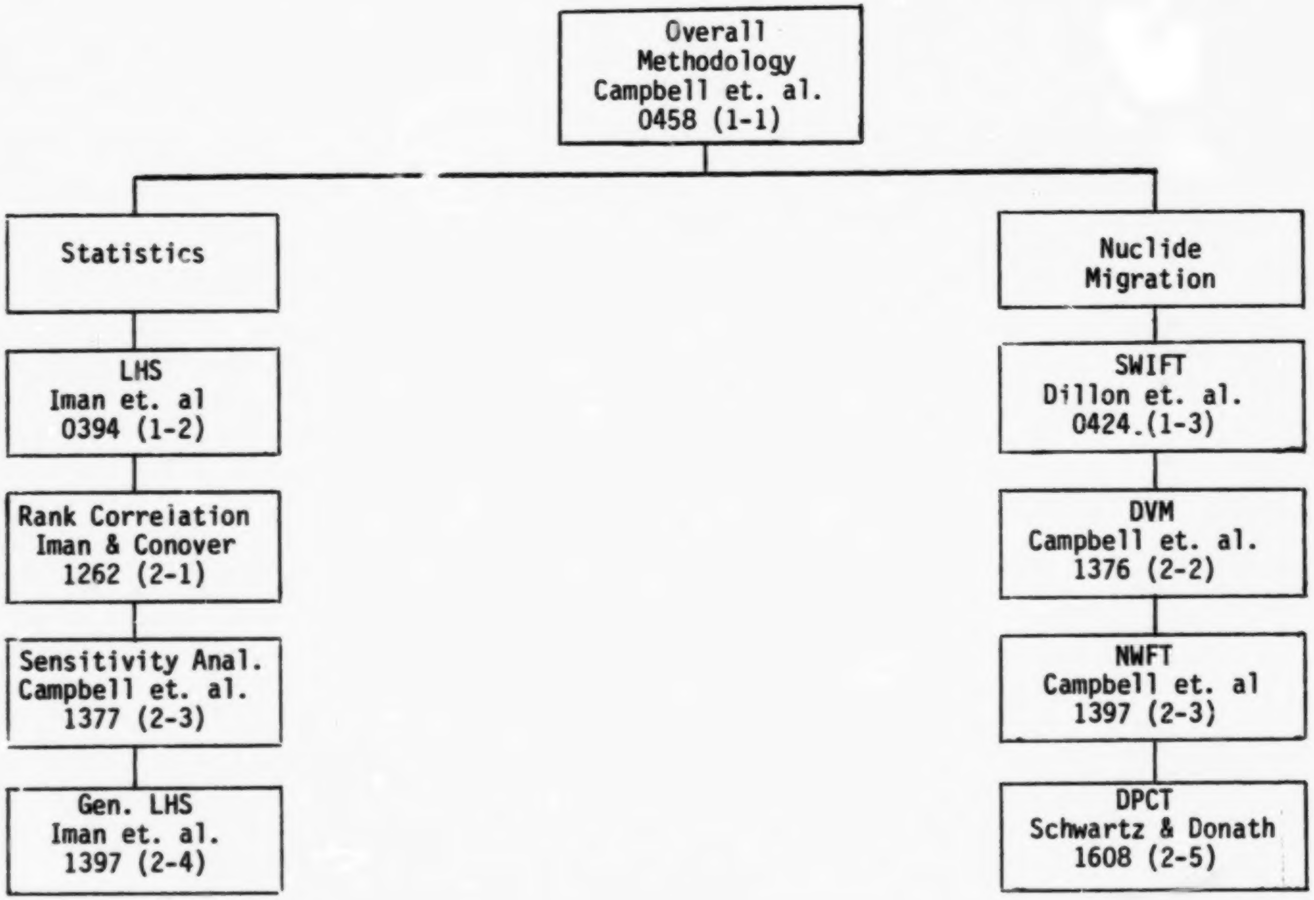


Figure 3-1

Taxonomy of the Risk Methodology that have been Reviewed

(4 digit number is last part of NUREG/CR-xxxx, first number in parenthesis is review phase number, second number is document number)

Changes in emphasis could also occur if the proposed 10CFR60 is implemented. For example, the work may very well focus on assuring that the waste packages would have zero release for the first 1,000 years and that the release rate from the repository is less than the prescribed rate. This could eliminate consideration of probabilities, biosphere transport, health effects, and presumably uncertainty and sensitivity analyses.

The above remarks tend to be critical of the work. This position stems somewhat from the nature of the review process and the ground rules. It must also be stated that a great deal of the work is innovative. Much has been done, for example, to advance the state-of-the art whereby uncertainties associated with nuclear waste repository risk can be dealt with.

3.2 Review of Individual Documents

3.2.1 Review and Critique of NUREG/CR-1262 (Document 1)

3.2.1.1 General Review

3.2.1.1.1 Summary

NUREG/CR-1262 begins with a review of two methods of inducing statistical dependence among several random variables. The methods mentioned include the formation of linear combinations of variables and the transformation of normal variates. A matrix method of inducing rank correlation among several variates is introduced. The authors claim that the latter method possesses the following properties:

1. The procedure is independent of the probability density function associated with the input variables,
2. It is simple,
3. It is applicable to any sampling scheme, and
4. The marginal distributions are unchanged.

3.2.1.1.2 General Comments

Prior to making specific statements regarding the content of NUREG/CR-1262, a few general remarks are in order. First, the development of a methodology for introducing some form of dependency among several random variables is a worthwhile objective. Whether or not rank dependence is the most appropriate form of dependence is a question that should be addressed. The authors fail to discuss, or even list, alternative measures of dependence. Discussion of these concepts may be found in Kruskal, W. H., Ordinal Measures of Association, J. Amer. Stat. Assoc., 53, 1958, pp. 814-861, Lehmann, et. al., "Some Concepts of Dependence," Ann. Math. Stat. 38, April 1967; Jogdeo, K., Patil, G.P., "Characterization of Independence in a Family of Bivariate Distributions with Regression Dependence," Ann. Math. Stat. 38, April 1967; and Barlow, R.E. and Proschan, F., "Statistical Theory of Reliability and Life Testing," Holt, Rinehart & Winston, 1975.

The second general remark has little or nothing to do with the methodology itself. The modeling of the dependency structure may be a purely academic exercise in light of the sparse amount of statistical data that is likely to be available regarding the physical processes in question. For example, the authors state, on the bottom of page 1, that significant correlations are expected to exist between hydraulic properties in the vicinity of a disposal site and the time for circulating groundwater to contact the radioactive waste. Although this may be true, it is doubtful that sufficient information will ever be available to actually estimate (quantitatively) the correlation between these variables. On the other hand, the methodology could be used to assess the importance (sensitivity) of such correlations.

3.2.1.1.3 Specific Comments

The overall structure or arrangement of the material in this report appears to be adequate. Unfortunately, the discussion is quite thin in the sense that most, if not all, of the results are presented without proof. Hence, it is difficult to verify the conclusions.

The inclusion of the list of properties in the introduction was a very good idea. Each of the four properties is presented in a clear and concise manner, with the exception of the third. An expanded discussion of property three should be given in Section 2 and reference to this discussion should appear within item three of the introduction. A simple example of how the given methodology may be used in conjunction with Latin hypercube sampling should be very helpful.

The authors state that their approach is based on the premise that rank correlation is a meaningful way to define dependencies among input variables. As stated above, this supposition brings to mind the question of why rank correlation was actually chosen as the measure of dependence. It is recommended that the authors discuss their choice and, as a minimum, list the various alternatives that are available.

Section 2, contains statements that are not clear. For example, the statement that begins on the bottom of page 4, "Let R be an N x K matrix whose columns represent K independent permutations of the integers from 1 to N." is confusing. First, there are N elements in each column of R, not K. This is apparently a typographical error. The term "independent" permutation is not clear. The authors probably mean random permutation, not independent permutation.

The mathematical results, stated on page 5, should be supported by proofs which may be relegated to an appendix. Alternatively, the authors should provide references to proofs when such references are known to exist. The Scheuer and Stoller paper does not show how the Cholesky factorization scheme was developed; one has to refer to the references given by Scheuer and Stoller. The need to trace through several references detracts from the paper's clarity and ability to stand by itself as an independent work.

3.2.1.1.4 Scope

The material presented in NUREG/CR-1262 concerns the problem of inducing rank correlation among sampled values of several input variables. The limitations of the method are not fully discussed by the authors.

3.2.1.1.5 Verification

As mentioned above, the mathematical results are stated without proof. This makes the task of assuring verification difficult.

3.2.1.1.6 Presentation

The presentation is very difficult to follow and the numerical examples do not assist the reader in understanding how the methodology may be used in conjunction with Latin hypercube sampling. Had sample numerical examples involving the LHS method been presented, the reader may have gained additional insight into the choice of rank correlation as a measure of dependence.

3.2.1.1.7 Report Conclusions

No conclusions are presented in the report.

3.2.1.2 Report Compared with Criteria

3.2.1.2.1 Model Realism

Not applicable to this report.

3.2.1.2.2 Methodology Validity

Mathematical results are stated without proof. Hence, validity of the results is left to the reader.

3.2.1.2.3 Data Validity

This criterion does not apply directly to this report. The numerical examples are presented for the purpose of demonstration and are not intended to be representative of an actual physical situation.

3.2.1.2.4 Time Period Appropriateness

The work presented here is not time dependent and hence this criterion is irrelevant.

3.2.1.2.5 Event Sequence Completeness

Not relevant to this report.

3.2.1.2.6 Key Parameter Identification

Not relevant to this report.

3.2.1.2.7 Uncertainty Analysis

Not relevant to this report.

3.2.1.2.8 Application of the Model for Licensing

The methodology presented in this report would be applicable to sensitivity and uncertainty analyses. Since the licensing requirements, as they exist or may be inferred, are not explicit on the need for uncertainty analysis, it is not possible to say just how the work relates to licensing.

3.2.2 Review and Critique of NUREG/CR-1376 (Document 2)

3.2.2.1 General Review

3.2.2.1.1 Summary

This report describes a simplified method for analyzing nuclide transport. The concept is based upon the fact that nuclide flow from a donor point to a receptor point, because of the many paths the flow may take, may be characterized by a distribution of velocities. The density of waste arriving at a point may be obtained by summing over all donor points. The solution to the equation expressing this summing process requires knowledge of the velocity distribution. Beginning with a Green's function solution of the dispersion flow equation, and using a transformation of variables, the desired velocity distribution is found to be Gaussian. In the numerical implementation, radioactive decay is introduced into the one-dimensional model. Results are compared with those obtained by an analytic solution as well as those obtained via finite difference methods.

3.2.2.1.2 General Comments

This report concentrates primarily on the development of what is purported to be a new method for treating convective-dispersive transport, namely the Distributed Velocity Method (DVM). Included in the report are discussions of the mathematical theory, numerical implementation, an error analysis, employing statistical sampling and regression analysis techniques, and comparisons of DVM with other methods for convective-dispersive transport.

In Chapter I, there is brief mention of other methods which are used for such analyses; however, the work of Ross and Koplik (5) whose publication also presents a new method for solving the transport equation is omitted. The work of Campbell, et. al., and that of Ross and Koplik share many similarities. A comparison of the two developments would have been desirable, especially since both were developed for performance assessment of a high-level radioactive waste repository, and both methods are based upon a Green's function approach.

Chapter II describes the theory underlying DVM. The derivations in this section are presented in a confusing manner, and the large number of typographical errors do not facilitate the readability of this report.

The model which is discussed is the standard convective-dispersion equation upon which practically all treatments of nuclide transport in an aquifer are based. The principal limitation of the model, as indicated by the authors, is that it is one-dimensional, and treats only a homogeneous or uniform dispersive medium and a constant aquifer velocity. Furthermore, no allowance is made for temperature-dependent and spatially dependent physical parameters. Such idealizations do not exist in the real world, of course, so the method is designed to obtain relatively rapid solutions to greatly simplified problems. This may be quite useful in broad parameter surveys; however, the method could be of limited value when assessing the adequacy of an actual site-specific repository.

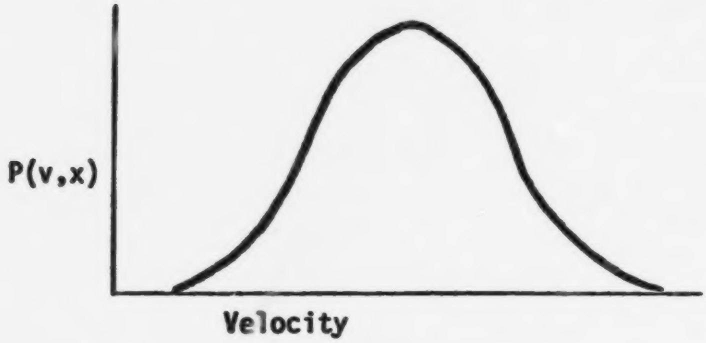
For simplicity of presentation, the discussion in Chapter II omits sorption and radioactive decay chains. This restriction is removed in the next chapter, entitled "Numerical Implementation." The generalization is first made for one decaying radionuclide, and then for a chain of radionuclides. Here, as before, the presentation is quite confusing. The diffusion equation to be solved, with the inclusion of radioactive decay, is never presented. A systematic method of solving the equation is not attempted. Instead, the first equation presented in this chapter is the solution:

$$\Delta\rho(i,j,t) = DW(j) \left\{ M(j)\, \rho(i-k_j,\, t') + [1-M(j)]\, \rho(i-k_j-1,\, t') \right\} \qquad (3\text{-}1)$$

This is followed by a lengthy, but vague, discussion devoted primarily to defining the terms in that solution. For example, a matrix B and a quantity N_B are introduced. It is stated that "Quantities $N_B(i)$ and $B(j)$ are most easily obtained by a computational procedure which makes the tests of Eq. (3-8) and accumulates the coefficients to form the B matrix." How this computational procedure is carried out is never explained.

The following overview of the theory follows the reasoning used in the report. The report begins with a phenomenological approach, but without knowledge of a specific velocity distribution. Recourse is then made to the solution of the dispersion equation, the result being a Green's function solution which yields the desired velocity distribution.

Consider an ensemble of particles at x' at time t' having density $\rho(x',t')$. Under convective transport the particles will pass point x at time t with a density $\rho(x,t)$. Because of the heterogeneity of the flow field, the particles move at different velocities; hence a velocity distribution $P(v,x)$, is visualized. The general form of $P(v,x)$ is illustrated below.



The density at x,t is obtained by summing over all possible donor points in the following manner

$$\rho_0(x,t,t') = \int_{-\infty}^{\infty} dv\, P(v)\rho(x',t'),$$

where v and x' are related by

$$v = (x-x')/(t-t').$$

If there is a source of particles $S(x',\tau)$ injected at time τ, then

$$\rho(x,t) = \rho_0(x,t) + \int_{t'}^{t} d\tau \int_{v_1}^{v_0} dv\, P(v)\, S(x',\tau) \qquad (3\text{-}2)$$

where the source term vanishes outside of the limits v_0 and v_1 and x_0 and x_1.

In order to carry out the integration the velocity distribution must be known. This could take many forms depending on the transport model. The velocity follows a Gaussian distribution if the model is a diffusion process. The authors essentially assume the latter process through recourse to the one-dimensional dispersion equation:

$$\frac{\partial \rho}{\partial x} = D\frac{\partial^2 \rho}{\partial x^2} - \bar{v}\frac{\partial \rho}{\partial x} + S \qquad (3\text{-}3)$$

which can be solved in the usual fashion by first replacing the arbitrary source S by the Dirac delta functions $\delta(x-x')\ \delta(t-t')$; that is

$$\frac{\partial G}{\partial t} = D\frac{\partial^2 G}{\partial x^2} - \bar{v}\frac{\partial G}{\partial x} + \delta(x-x')\ \delta(t-t') .$$

It can be shown, using Laplace transforms for example, that the solution to this equation yields the Green's function

$$G(x,x',t,t') = \frac{1}{\sqrt{2\pi}}\ \frac{1}{\sqrt{2D(t-t')}}\ e^{\frac{-[(x-x') - \bar{v}(t-t')]^2}{4D(t-t')}} \qquad (3\text{-}4)$$

The solution of Equation (3-3) can now be expressed in terms of this Green's function as follows:

$$\rho(x,t) = \iint S(x',t')\ G(x',x,t,t')\,dx'dt' \qquad (3\text{-}5)$$

or

$$\rho(x,t) = \frac{1}{\sqrt{4\pi D}} \int_0^t \frac{dt'}{\sqrt{t-t'}} \int_{-\infty}^{\infty} dx' e^{\frac{-[x-x'-\bar{v}(t-t')]^2}{4D(t-t')}} S(x',t') . \quad (3\text{-}6)$$

It is possible to obtain an equation which appears more concise by changing variables from x' to v where v is defined by

$$v = \frac{x-x'}{t-t'} \quad (3\text{-}7)$$

The new variable v has the dimensions of velocity and can be thought of as an effective velocity of a particle arriving at (x,t) having been located at x' at the earlier time t'. Since particles, which may all be traveling with the same speed, can pursue a wide variety of paths in arriving at the position x from x', they will in general arrive at different times and thus, according to Equation (3-7), have different effective velocities.

Making the change of variable indicated in Equation (3-7), Equation (3-6) becomes

$$\rho(x,t) = \frac{1}{\sqrt{4\pi D}} \int_0^{t'} \sqrt{t-t'}\, dt' \int_{-\infty}^{\infty} dv\, e^{-\frac{1}{4D(t-t')}\left[(v-\bar{v})\ (t-t')\right]^2} S\left(x-v(t-t'),\ t'\right). \quad (3\text{-}8)$$

If we define σ_v as follows

$$\sigma_v = \sqrt{\frac{2D}{(t-t')}} \quad (3\text{-}9)$$

equation (3-8) may be rewritten as

$$\rho(x,t) = \int_0^t \frac{dt'}{\sqrt{2\pi}\ \sigma_v} \int_{-\infty}^{\infty} dv\ e^{\frac{-(v-\bar{v})^2}{2\sigma_v^2}}\ S\left(x-v(t-t'),t'\right) . \quad (3\text{-}10)$$

Defining the quantity

$$\bar{G}(v,t-t') = \frac{1}{\sqrt{2\pi}\,\sigma_v}\; e^{-\frac{(v-\bar{v})^2}{2\sigma_v^2}} \tag{3-11}$$

leads to the relationship

$$\rho(x,t) = \int_0^t dt' \int_{-\infty}^{\infty} dv\; \bar{G}(v,t-t')\; S\Big(x-v(t-t'),t'\Big) \tag{3-12}$$

which makes it reasonable to think of $\bar{G}(v,t-t')$ as a Green's function in velocity space, corresponding to the velocity density, $P(v)$, in Equation (3-2).

It would have been helpful if the authors had written the solution for the density ρ in terms of the Green's function; thus, using their notation and including the decay term,

$$\rho(x,t) = \int_0^t dt' \frac{e^{-\lambda(t-t')}}{\sqrt{2\pi}\,\sigma_v} \int_{-\infty}^{\infty} dv\; e^{-\frac{(v-\bar{v})^2}{2\sigma_v^2}}\; S\Big(x-v(t-t'),t'\Big), \tag{3-13}$$

where

$$\sigma_v = \sqrt{2D/(t-t')}\ .$$

Also, the authors should have explained in a systematic way how the integrand was discretized in order to perform the numerical integration. There are many ways to do this and the report does not adequately explain what was done. Instead, the reader is referred to Figure 2 and is informed that, according to the figure, "there are, in general, two contributions to receiver block i...". What relation the figure has to the required integration is certainly not clear. Why, for example, are there only two contributions to receiver block i? For a distributed source, why aren't there more? In fact, because of dispersion, some of the donor blocks could, in principle, be downstream (>i) as well as upstream. The explanation could have been made for a parent nuclide, for which S represents the amount of that nuclide leaving the repository. In addition, it could have been done for daughter products, for which S would represent the amount leaving the repository plus the amounts produced by precursors in transit.

In the discussion dealing with a chain of radionuclides, equations to be solved are omitted. The solutions, as before, are stated rather than derived. This contributes to a great deal of confusion. Consider, for example, the statement "In this equation $\Delta\rho$ is the incremental particle density for isotope r, grid block i, velocity subgroup j, and time t which arises from decay of isotope r-p. If p=0, Equation (3-10) degenerates to Equation (3-1)." Now Equation (3-1) is the solution for one decaying nuclide, while the case p=0 implies a decay from isotope r to isotope r. While it is not clear what would be meant by the latter, it is not apparent that it implies decay by one radionuclide.

The assertion that the Bateman equations describe the production and decay of radionuclides for the present application requires some justification. While it is true that these equations represent the correct solution in a space-independent context, their seemingly arbitrary use in the present space-dependent situation certainly deserves some explanation or discussion. What manner of approximation permits the use of a space-independent result to this one-dimensional computation? The authors assert the accuracy of their model by citing two example calculations; however, this is not sufficient.

The error analysis presented in Chapter IV is interesting. It differs from conventional techniques, and makes use of Latin hypercube sampling, a subject which is a principal theme throughout most of the Sandia reports. Insofar as it goes, the analysis which is presented is rather thorough. However, as the authors state, all of their attention is devoted to a one dimensional flow problem and, within that, it is restricted to one point in space, namely a point 100,000 ft from the donor point. Other distances could conceivably lead to conclusions which are different from those reached by examining just the one distance.

One of the conclusions reached by the authors reads as follows, "numerical error may be decreased and, at the same time, the technique may be made more efficient by simply increasing the time step." This conclusion seems astonishing to those familiar with standard numerical methods. It also suggests the question, "Why don't we solve any given problem with just one large time-step?" Surely something is missing relative to the discussion of accuracy versus time step size.

In spite of the above comments, the DVM method appears to offer a new and, in some cases, more efficient method of evaluating radionuclide transport. A clearly written explanation of how it works is still missing, however.

3.2.2.1.3 Scope

The scope of the work presented here is quite limited. Its purpose is to describe the distributed velocity method (DVM), implement it, analyze the errors associated with the numerical implementation and compare results with analytic and finite difference solutions of the nuclide transport equation. The method, in its present form, is limited to one dimension.

3.2.2.1.4 Verification

Results from DVM are compared with the method of characteristics with GETOUT (6), with SWIFT (7) and with analytic solutions. The agreement of all methods with each other is excellent, but not all code alternatives are being exercised and the decay is a simple isotopic decay (isotopes not identified).

3.2.2.1.5 Presentation

The presentation has been discussed under the General Comments (Section 3.2.2.1.2).

3.2.2.1.6 Report Conclusions

The conclusions of this report are that the DVM method exhibits computational efficiency, the ability to handle decaying radionuclide chains with highly contrasting solution velocities and the ability to treat both solution and leach-limited sources. Within the testing that has been performed the DVM appears to meet these requirements.

Not all of these features have been tested; however, the code is probably able to treat the problems within its one-dimensional capabilities since it is basically a Green's-function solution of the nuclide transport equation, a method that has been highly developed by others, e.g., Ross and Koplik (5).

3.2.2.2 Report Compared With Criteria

3.2.2.2.1 Model Realism

The model used here is realistic but limited in applicability. It is suspected that the extension to multi-dimensions would slow the computational speed to the point that the DVM method would lose its usefulness. It is limited to homogeneous media whereas repositories may be placed in stratified media. Should heterogeneous calculations be necessary, a code such as that of Hadermann (8) is suggested.

3.2.2.2.2 Methodology Validity

The validity of the methodology is subject to the remarks in Section 3.2.2.1. Although the methodology has been compared to analytic solutions as well as SWIFT and GETOUT calculations, such comparisons do not fully validate the methodology.

3.2.2.2.3 Data Validity

The data used in this report are not valid. The data are only intended to demonstrate the model.

3.2.2.2.4 Time Period Appropriateness

The time period is apparently 10^8 years which is quite adequate to encompass the repository lifetime.

3.2.2.2.5 Event Sequence Completeness

The event sequences are not complete. This report assumes the repository fails, assumes a leach time and calculates the release rate from its boundaries.

3.2.2.2.6 Key Parameter Identification

This report does not include a sensitivity analysis; hence there is no key parameter identification.

3.2.2.2.7 Uncertainty Analysis

This report does not include an uncertainty analysis.

3.2.2.2.8 Application of the Model for Licensing

This model could be appropriate for licensing if the repository has a simple enough geometry that it may be treated by DVM. The output appears to be appropriate for licensing since it is stated in terms of release rates. However, one must account for the fact that the canister release rate for the first 1,000 years must be zero.

3.2.3 Review and Critique of NUREG/CR-1377 (Document 3)

3.2.3.1 General Review

Summary:

The purpose of the work reported in NUREG/CR-1377 is to determine the relative importance of hydraulic and geochemical variables which may influence radionuclide migration in groundwater. The report contains:

(1) A comparison of two finite difference models of groundwater flow and

(2) A demonstration of several statistical procedures* used in the sensitivity analysis of the computer generated data.

In addition, the report contains: (1) a review of some sensitivity analysis techniques, (2) a definition of the reference site, (3) a comparison of results using the SWIFT model (presumed to be accurate) and the Network Flow and Transport (NWFT) model (a one-dimensional model), and (4) a discussion of three scenarios, namely a U-Tube with river discharge, a U-Tube with well discharge and a hydraulic connection between overlying and underlying aquifers. The site is the same one that has been used in NUREG/CR-0458 (Campbell et. al.).

Because of the complexity of the SWIFT model, the desirability of a simpler model with which to perform sensitivity analyses was apparent. Hence, the NWFT model was developed. The authors suggest that NWFT is adequate for sensitivity studies despite the fact that there are many phenomena which NWFT cannot model. For the solubility-limited case the important variables are the solubility-limit and the distribution coefficient. For the leach-limited case, the important variables are leach time and the distribution coefficients.

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*The statistical procedures include response surface techniques, Latin hypercube sampling and the use of the rank transformation.

3.2.3.1.1. General Comments

Because it utilizes much of the statistical machinery developed by Sandia, this document should be written in a manner that facilitates understanding by those who may not be specialists in the subjects addressed. In light of this, the following have been set down as key requirements in the current review:

(1) A clear and concise statement of the problem or purpose of the study,

(2) A description of the underlying assumptions and limitations of the methodology,

(3) A discussion of the underlying assumptions and limitations of the methodology,

(4) A clear statement of the results, including an interpretation of any mathematical results that might be considered, in some sense, abstract, and

(5) A discussion of the capabilities of the methods relative to other approaches that might have been taken.

Along the lines of report organization, the abstract describes the general purpose of the study and what was done; it does not mention any of the findings or conclusions. A brief summary of the findings and conclusions would be beneficial. A one page executive summary enumerating the conclusions also would have been useful.

The review of sensitivity analysis techniques presented in Section 2 was a good idea. However, with the exception of the discussion of Latin hypercube sampling (LHS), the review appeared to be incomplete. The authors assumed familiarity with the LHS technique and rank transformation, although these are not standard statistical procedures. Little is known, or at least published, regarding the performance of LHS when applied to non-monotonic functions, a point raised in the Phase I review (Volume 1 of NUREG/CR-1672).

It is the understanding of the reviewers that monotonicity is a sufficient condition that ensures greater efficiency of the LHS method over that of random sampling. If the LHS method is not robust, i.e., does not work well when applied to non-monotonic functions then the use of LHS may impose an unnecessary restriction on the analysis.

The authors assume that all readers, including those that do not have a great deal of experience in the application of regression analyses, have a feeling for the difficulties inherent in non-linear regression. They should be very explicit about their reasons for recommending the rank transform. Perhaps a brief summary of the material contained in the authors' paper which appeared in Technometrics Vol. 21, November 1979, would be appropriate.

A serious problem can occur if a reader with some background in statistics interprets the results of the rank regression analysis as though the regression was based upon the raw data. The authors should be very explicit about the fact that extrapolation cannot be done with rank regression. If it is necessary, or desirable, to obtain a mathematical relationship between the variables, rank regression is not appropriate. The reviewers feel that the uninformed reader may try to interpret the results of the regression on the ranked data as though they were dealing with a typical regression model. The same holds for the interpretation of the coefficient of determination, R^2. What does it really mean if one obtains a high value of R^2? It is well known, in fact documented in the Technometrics article referred to above, that one can obtain a high value of R^2 when applying regression to ranked data yet very small values of R^2 may occur when applying regression to the raw data. All of these issues should be clearly presented.

When comparing the results of the NWFT code with the results of the SWIFT code, as in Figures 10, 12 and 13, it would be useful to include confidence intervals on the empirical distribution functions. This would allow the reader to determine whether or not the differences are statistically significant. The Kolmogorov-Smirnov statistic provides a very convenient way of constructing such an interval (see for example, Hoel, P.

Introduction To Mathematical Statistics, or Massey, F. J. The Kolmogorov-Smirnov Test for Goodness of Fit, J. Am., Stat. Assoc., March 1951). However, the use of the LHS technique seems to preclude the use of the Kolmogorov-Smirnov statistic.

Another comment is that the results are not to be taken literally. No allowance is made for the time for water to reach the canisters nor for the time at which canister failure occurs. This omission may result in a significant error in the radionuclide decay calculations. More activity may be predicted at the time of release than would actually occur if the delays were properly accounted for.

A further comment is that the variables selected for the sensitivity analysis are not the only variables that enter the problem. The hydraulic pressure and groundwater velocity may enter as strongly as k_d.

There are several minor deficiencies that serve to confuse the reader; for example, typographic errors such as $x_{10}\ x_{14} = K_s/\phi_s$ which should be corrected to read $x_{10}\ x_{14} = K_s/\phi_s\tau$ in Table 3, page 32, and undefined terms such as "dip angle" that appears on page 47.

3.2.3.1.2. Scope

The work presented here is quite limited in scope. It appears to have three purposes:

1. Demonstrate the application of LHS and stepwise rank regression to SWIFT and NWFT.
2. Conclude that sensitivity results obtained via the NWFT code correspond with the sensitivity results obtained via the SWIFT code.
3. Demonstrate sensitivity analyses using NWFT on three waste repository disruption scenarios.

The report makes little pretense at rigor in justifying the use of LHS or stepwise rank regression but concentrates on the above objectives.

3.2.3.1.3. Verification

The verification consists of the comparison of sensitivity results using the SWIFT and NWFT codes. This is not a very rigorous test since it does not test the full range of parameters in either code. Furthermore, sensitivities are determined by the same method in both cases. Better tests in this regard are presented in Document 4.

3.2.3.1.4. Presentation

Sufficient comments on the presentation have already been made. It could be improved.

3.2.3.1.5. Report Conclusions

The conclusion that sensitivity studies may be performed using the NWFT code instead of the more accurate but slower SWIFT code have not fully been demonstrated because all of the variables have not been exercised.

It should be borne in mind that a sensitivity analysis is not the end product. The end product in this case is an uncertainty analysis of the repository performance. This document does not take this last step.

3.2.3.2 Report Compared with Criteria

3.2.3.2.1. Model Realism

The NWFT model may be limited in applicability. Also, the conclusions, as presented, may be subject to misinterpretation.

3.2.3.2.2 Methodology Validity

The validity is subject to the remarks of Section 3.2.3.1. The method seems to be sufficiently valid, given the uncertainties in model parameters (i.e., order of magnitude validity).

3.2.3.2.3 Data Validity

The data used in this report were used for purpose of exposition. No claims have been made relative to the validity of the data.

3.2.3.2.4 Time Period Appropriateness

The time period is one-million years, which seems adequate.

3.2.3.2.5 Event Sequence Completeness

The event sequences are not complete nor is there any claim to completeness.

3.2.3.2.6 Key Parameter Identification

The primary objective of the report is to identify the key parameters. It should be noted, however, that the identification of the key paramterers depends on the acceptability of the scenarios selected.

3.2.3.2.7 Uncertainty Analysis

The sensitivity analysis is not extended to the point where the numerical results include confidence estimates.

3.2.3.2.8 Application of the Model for Licensing

The proposed 10CFR60 does not explicitly require sensitivity analyses or uncertainty analyses; hence, the relevance of this work to licensing is not clear.

3.2.4 Review and Critique of NUREG/CR-1397 (Document 4)

3.2.4.1 General Review

Summary

The major new contribution of this volume is the generalization of Latin hypercube sampling (LHS) to allow for strata with unequal probability size or content and the estimation of model output when the distributions of the input variables have been perturbed slightly. The generalization is developed theoretically, demonstrated in an example and applied to the calculation of groundwater flow using the NWFT model. The report addresses many important questions such as the identification of influential input variables, the effect on the output caused by assumptions regarding the input distribution functions and the effect of sample size on the estimated cumulative distribution functions. This report also provides a comparison between LHS, random sampling and replicated LHS. The report ends by illustrating the usefulness of generalized LHS in the comparison of scenarios.

3.2.4.1.1 General Comments

This document is valuable in that it provides an over-all perspective regarding the emphasis in the Sandia program on the statistics of sampling. If this discussion had appeared in a central program overview discussion, such as Campbell et. al. (NUREG/CR-0458), a considerable amount of confusion may have been eliminated. The following qualitative discussion is provided to assist the reader in understanding the reasons for mathematical methods being developed in the program.

A basic problem confronting the Sandia group doing this work is that the mathematical model of the repository is numerical rather than analytic. Furthermore, it is not possible to pin-point a specific object or piece of coding as the model; rather, the model is actually a composite of several codes which will ultimately be linked together plus side calculations and judgments that may be made by specialists. The input to such a model must take the form of a discrete set of numbers. In one approach, the best estimates of these numbers are used. Alternatively, the values assigned to the input variables may be selected from a range of values which are representative of the actual geophysical situation being modeled, the selection being in accordance with a given probability distribution. In addition to the uncertainty of the values chosen, the input variables, in fact, may be correlated or associated in some way.

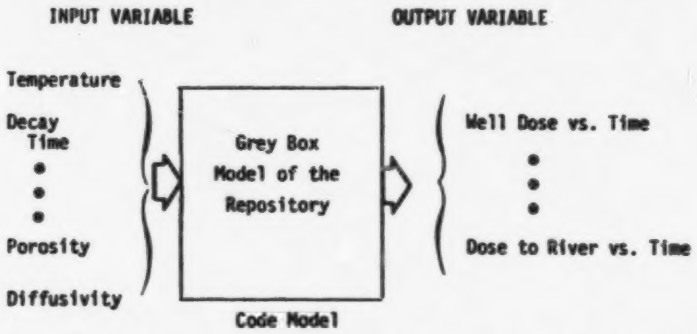

Figure 3.2. Conceptualization of the Waste Repository Modeling.

The numerical model is represented by a so-called grey box, Figure 3.2, in that it is possible to look inside and examine individual steps; however, the complexity defies comprehension. As a result of this, the model may be thought of as a black box into which certain input information is fed and certain output information is extracted. If the model is exercised many times, each time with input values selected from a distribution, the results of the model will be distributed in some way. Such a distribution defines the likelihood of different model predictions.

Unfortunately, a considerable amount of computer time may be required in order to obtain a single solution for a given set of input parameters. This makes it impractical to randomly sample from each input distribution to construct the output distribution because of the large number of calculations necessary to encompass the input distributions.

The Sandia group has developed and applied a statistical technique called Latin hypercube sampling (LHS), which is a generalization of Latin square sampling. It is asserted that LHS may be used to characterize the output distribution with fewer calculations (smaller sample size) than would be needed if other sampling schemes were used. Indeed, the authors suggest that with hundreds of inputs, the output distribution can be determined on the basis of only 50 to 100 runs.

The following is a restatement of Latin hypercube sampling (LHS) method and the generalization presented in this report:

A sampling procedure called Latin hypercube sampling (LHS) has been described by McKay, Conover and Beckman*. LHS is essentially a K-dimensional generalization of Latin square sampling**. The support*** of each of K variates, x_1, x_2, ..., x_k, is partitioned into N disjoint intervals. The K-tuple of input variables $\underset{\sim}{X} = (x_1, x_2, \ldots, x_k)$, may be visualized as a point in a K-dimensional vector space. With this in mind a Latin hypercube sample may be described as a set of N points located in a K-dimensional space in such a way that each of the intervals associated with the variates is represented exactly once in the collection of sample points. A two-dimensional example is given in Appendix D (see page D-8 of this report).

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*Technometries, 21, 239-245.

** McKay, M., Conover, W., and Whiteman, D., Informal Report LA-NUREG-6526-MS.

*** A density function f and its distribution F are concentrated on an interval I if f(x)=0 for all x outside I. The smallest closed interval I with this property is called the support of f.

Let $\underset{\sim}{X}_1, \underset{\sim}{X}_2, \ldots, \underset{\sim}{X}_N$ represent N sample points. Each of these points, or K-tuples, describes the set of values assigned to K input variables of a computer simulation code. The output which corresponds to each of these input sets will be denoted $Y_1, Y_2, \ldots Y_N$, respectively. The simulation which establishes the correspondence between Y_j and $\underset{\sim}{X}_j$, j=1, ..., N, may be thought of as an unknown, although observable function of the input variables; i.e., the simulation defines the function $Y = h(\underset{\sim}{X})$. The LHS procedure ensures that each of the input variables, $x_1, x_2, \ldots, x_k$, is represented in a fully stratified way regardless of whether or not the output, Y, is dominated by any subset of the input variables. In the McKay, Conover, and Beckman paper referred to above, the support of each of the K input variables was partitioned into N intervals each having probability size 1/N.

The statistic $T(Y_1, Y_2, \ldots, Y_N) = \frac{1}{N} \sum_{i=1}^{N} g(Yi)$ is used as an estimator for the moments of Y. For example, the estimator for the r^{th} moment of Y is given by the statistic

$$Y(Y_1, Y_2, \ldots, Y_N) = \frac{1}{N} \sum_{i=1}^{N} Y_i^r$$

when g is the indicator function defined as follows

$$g(Y) = \begin{cases} 1 \text{ when } Y \leq y \\ 0 \text{ otherwise,} \end{cases}$$

the statistic $T(Y_1, Y_2, \ldots, Y_N)$ becomes an estimator for the cumulative distribution function of Y.

If $Y = h(\underset{\sim}{X})$ is monotonic in each of the variables $x_1, x_2, \ldots, x_k$ and g(Y) is a monotonic function of Y, then the variance of the statistic $T(Y_1, \ldots, Y_N)$ derived via Latin hypercube sampling will be smaller than the variance of $T(Y_1, \ldots, Y_N)$ derived via random sampling. This is the result previously presented (NUREG/CR-0394).

In the present report (NUREG/CR-1397) the LHS method is generalized in the following way. The support of the K input variables is partitioned into N intervals, say

$$\begin{array}{l} I_{1,1},\ I_{1,2},\ldots,I_{1,N} \\ I_{2,1},\ I_{2,2},\ldots,I_{2,N} \\ \cdot \quad\quad \cdot \quad\quad \cdot \\ \cdot \quad\quad \cdot \quad\quad \cdot \\ \cdot \quad\quad \cdot \quad\quad \cdot \\ I_{K,1},\ I_{K,2},\ldots,I_{K,N}, \end{array}$$

each of probability size

$$p_{k,n} = P\left[x_k \varepsilon I_{k,n}\right] .$$

Under the assumption of statistical independence, the probability size of each of the N^k cells, into which the entire space of input variables has been partitioned, is given by the product

$$p_n = p_{i,n_1} \cdot p_{2,n_2} \cdot\cdots\cdot p_{K,n_K} ,$$

where n represents the K-tuple $(n_1,n_2,\ldots,n_k)$ which identifies a particular cell. In other words, the probability size of the individual cells is no longer uniformly distributed with value 1/N assigned to each cell. The statistic $T(Y_1,Y_2,\ldots,Y_N)$ has been modified as follows

$$T(Y_1,Y_2,\ \ldots,Y_N) = \sum_{i=1}^{N} N^{K-1}\ p_{\underset{\sim}{n}_i}\ g(Y_i) .$$

The authors show that E[T] = E[g(Y)]; in other words, T, as defined above, is an unbiased estimator of g(Y). This is, of course, a very nice result. The authors also show how a change in the weights which appear in T, can account for small changes in the distributions of the input variables.

In commenting on the mathematics, and clarity of presentation, we would like to state that the derivation and presentation of the mathematical results are, in general, not as clear as they should be. Lack of adequate examples, the use of somewhat complicated notation, and the absence of sufficient mathematical detail in the proofs contribute to the lack of clarity. A specific example of this is given in Appendix D of this report, where the proof of the key theorem in NUREG/CR-1397 is rewritten. Vague statements or terms abound; examples include: "usually smaller", "may be closely related", "reasonably smooth", "under usual circumstances". A number of typographic errors also make the reading somewhat difficult.

The section which describes a specific application of LHS suffers from lack of clarity also. Tables containing a large collection of numbers appear without much explanation. The reader's attention should be directed toward specific entries in these tables which illustrate a given feature or point the authors are trying to illustrate.

It is recommended that the LHS method be applied to a set of simple, although illustrative, problems for which the results are known. For example, why not take advantage of the fact that several distributions are self-replicating under certain types of algebraic operations? It is well known that the Gaussian distribution results when linear combinations of independent Gaussian random variables are formed. The lognormal is self-replicating under multiplication. The gamma and beta distributions also exhibit certain invariance properties under addition and multiplication, respectively. Therefore, simple functions of K input variables, e.g.,

$$Y = \alpha_1 X_1 + \alpha_2 X_2 + \ldots + \alpha_K X_K$$

or

$$Y = X_1^{\alpha_1} X_2^{\alpha_2} \ldots X_K^{\alpha_K}$$

could be used to demonstrate how well the LHS method really works. In the first case, the linear combination of X_j's, Y will be Gaussian provided the X_j's are independent Gaussian distributed random variables. In the second case Y will be lognormal if the X_j's are lognormal.

It is virtually impossible to judge how well the LHS method works when applying it to a reference site such as that used in NUREG/CR-1397. The so called "true" distribution functions which appear in NUREG/CR-1397, are no truer than any of the others which appear in the report. There is no way to obtain the actual distribution function with which to compare the empirical distributions derived via the LHS method. The only way to really validate the LHS method appears to be through the use of an artificial example for which the answer is known a priori.

The work is technically correct as far as this review has revealed, however, it is felt that the limitations of the LHS method have not been completely examined. For example, relaxation of the requirement for monotonicity (a sufficient condition) has not been explored. It may well be that the LHS method works well when the monotonicity property does not hold.

The comparison between LHS, replicated LHS and Monte Carlo sampling was a very good idea. Generally the Sandia work suffers from a lack of comparison with the work of others. Such comparisons would tend to strengthen confidence in the work.

There is some concern among the reviewers that there is a tendency to try to increase the uncertainty range of some input variables to unrealistic limits in order to span the space between realistic and conservative values. Having observed the results of this report and Sandia's previous reports in which LHS, sensitivity analysis and ranking of input variables were discussed, there is the possibility that a large range will result in an increase in the variable's ranking over the rank it would have had if known with less uncertainty. This should be explored to assure that the ranking is not an artifice of the uncertainty bound.

3.2.4.1.3 Scope

The scope of the work includes the development, presentation and demonstration of generalized LHS. The scope should have included an exploration of the limitations of LHS.

3.2.4.1.4 Verification

Verification of the mathematical results has been hampered to some extent by the lack of clarity of the presentation. It is recommended that the LHS method be applied to a variety of simple examples for which the results, i.e., the moments of Y and the distribution of Y are known or can be derived analytically. Having demonstrated that LHS works well when applied to simple examples, of course, does not constitute a proof or demonstration of its applicability to real world problems. However, one's confidence in the method may be bolstered by such a demonstration.

The verification presented here is a comparison of sensitivity analyses performed using LHS, replicated LHS and Monte Carlo sampling. For purposes of scenario comparisons, it is not obvious that any sensitivity analyses are necessary and the comparisons may be performed using expected values of the variables.

3.2.4.1.5 Presentation

Comments regarding the lack of clarity of this report have already been made. Detailed comments may be found in Appendix D.

The presentation in the report is of mixed quality. It is suggested that the mathematical generalization of LHS (GLHS) be relegated to an appendix and the results simply stated in the text. This would smooth the flow to the presentation of the demonstration of applications of GLHS and tests against other sampling procedures. The method has limitations that are not discussed in the report and the report would benefit from a full exploration.

3.2.4.1.6 Report Conclusions

The report conclusions are not well summarized. Generalized Latin hypercube sampling may be a very useful tool; however, the facts which support the argument in favor of LHS have not been presented very well. The results of GLHS appear to be superior to those obtained with Monte Carlo methods in the comparisons presented here. A sample size of 100 to 200 is sufficient when there are 14 input variables. Much smaller samples may be used for scenario comparisons.

3.2.4.2 Report Compared with Criteria

3.2.4.2.1 Model Realism

This criterion is not directly applicable to this report. This report concerns the generalization of the LHS method and, as such, involves the investigation of certain mathematical properties of LHS, not primarily the modeling of physical phenomena. In the modeling presented, the nuclide transport model used here is one dimensional and not intended to be particularly realistic. The GLHS methods are correct if subjected to the proper constraints but such constraints may not allow the determination of the most important measures of repository performance.

3.2.4.2.2 Methodology Validity

The methodology appears to be valid; however, a great deal more needs to be done with respect to the investigation of the limitations of the LHS method.

3.2.4.2.3 Data Validity

The data are consistent with Campbell et. al. (1) however, the data used here is more for illustrative purposes than a serious attempt at repository analysis.

3.2.4.2.4 Time Period Appropriateness

The time period chosen for the illustrative example is 10^6 years and hence appropriate, however, the results are cumulative over this period.

3.2.4.2.5 Event Sequence Completeness

There is no attempt to achieve completeness - the report aims at methodology demonstration.

3.2.4.2.6 Key Parameter Identification

This is a primary purpose of the work presented here although key parameters are not identified in the example.

3.2.4.2.7 Uncertainty Analysis

One of the limitations of LHS is the fact that standard goodness of fit criteria may no longer apply.

The statistic $T(Y_1,Y_2,\ldots,Y_N)$ has been shown to be an unbiased estimator of $E\{g(Y)\}$. However, there are other properties of $T(Y_1,Y_2,\ldots,Y_N)$ which must be considered. For example, it would be nice to know something about the distribution of T. Also, it would be nice to obtain interval estimates of the moments of Y and/or confidence intervals on the distribution function of Y.

3.2.4.2.8 Application of the Model to Licensing

The primary thrust of this report is that of performing sensitivity and error analyses using certain uncertainties in the input data to the NWFT code. In this sense its application is not apparent because 10CFR60 does not require sensitivity or error analyses.

3.2.5 Review and Critique of NUREG/CR-1608 (Document 5)

3.2.5.1 General Review

3.2.5.1.1 Summary

This report presents two dimensional analyses of two types of repository disturbances: (1) a vertical zone of higher or lower conductivity than the surrounding media for a bedded salt repository and (2) uniformly distributed fractures in a massive rock unit such as in a granite repository.

The calculation of these disruptive events is through the use of the deterministic-probabilistic contaminant transport code (DPCT). The ground water flow field is first determined; this is the deterministic part. Dispersion is then introduced by adding a random component to the deterministic part. It should be noted that the probabilistic part of DPCT has nothing to do with the probability of a geologic geometry existing at a future time nor the probability of a disruptive event. The results of 25 cases are presented.

One conclusion of this study was that a high conductivity zone has a localized effect on the flow patterns while a low conductivity zone can produce dramatic changes in the ground water flow field and influence the flow field across the entire section. This conclusion is not surprising. The effect of a high conductivity intrusion is essentially the same as if the intrusion were not present, i.e., ready flow across the vertical intrusion. The effect of a low conductivity (high impedance) intrusion is, in two dimensions, to block the flow from one side to the other. The effect should be less dramatic in three dimensions.

3.2.5.1.2 Comments

This report is well written and well organized. There are many simplifying assumptions in formulating the transport problem. Some terms such as degeneration with time and interaction with porous media are included in the formulation of the model but not used in the actual simulation. Some of the assumptions like isothermal flow (page 5, last paragraph) are not correct.

Hydraulic properties for geologic units comprising the RRS in bedded salt which appear in Table 2.1 and Appendix A are the same as those in an earlier report by Sandia (SAND 78-1267) which was reviewed during Phase I. The rock properties used in the previous report as well as the present report do not seem to be very realistic. Whether or not salt can be treated as a porous medium is a question that remains to be answered.

For example, a conductivity of 10^{-6} ft/day is equivalent to about 3.66 x 10^{-6} darcy permeability; i.e., about 4 micro-darcy. Darcy's law, which is used in the formulation, may not be valid at such low permeability. The flow may be more a slip flow or molecular diffusion at such low permeability. The Klinkenberg effect and the electrokinetic effect may be substantial; hence Darcy's equation will no longer be valid. In addition, porous media which have a permeability of a few millidarcy are considered extremely tight.

In the discussion of the results the authors make the following statement, "flow in the disposal unit is strongly influenced by small changes in hydraulic conductivities at initial locations in the flow system." This observation is in accord with common sense and practical experience. The selection of appropriate values of hydraulic conductivities for the different rock types is therefore key to the overall analysis. The values of hydraulic conductivities used in the RRS for both salt and granite appear to be very high, i.e., unnecessarily conservative. This will have a large effect on the results and conclusions drawn.

In attempting to justify their treating bedded salt as a porous medium, the authors state, on page 8, that "this assumption provides a conservative result which, *in itself*, justifies such a treatment for the purpose of assessing the risks in the isolation of nuclear waste." Unfortunately, it appears that the authors have applied this kind of faulty logic in making a large number of conservative assumptions, to the extent that one questions the validity of the results in a real repository setting. The authors should have been aiming for realistic assumptions and properties which, *if anything*, err on the side of conservatism. They should not have deliberately made conservative assumptions; it is the role of "probabilistic" modeling to account for variations in the input data and uncertainties in the modeling.

Due to the conservative assumptions, the "absolute" numbers resulting from the analyses should not be taken too seriously. For example, although it is valuable as part of a sensitivity analysis to locate the repository within a disruptive zone, this should never occur in practice; therefore, it is not a realistic scenario.

Also, as the authors state in the "Discussion," the results are highly dependent on the RRS chosen (i.e., geometry, geology, rock properties and hydrology of the hypothetical site chosen for analysis). This is another reason why general conclusions about repositories in salt should not be drawn from this study. Several other reference repository sites and scenarios should be analyzed before such conclusions can be made.

It should be stated that there are numerous failure mechanisms associated with repositories in bedded salt; these include:

a. Natural Causes

- Meteorite impact
- Climatic changes, such as glaciation, and innundation by sea water following a warming trend
- Flooding of repository during the operational phase
- Dissolution by circulating ground water; e.g., single connection to an aquifer, double connection to an aquifer, connection between two aquifers through the salt deposit
- Fluvial erosion
- Volcanism
- Earthquakes, seismicity and faulting

b. Man-made Causes

- Sabotage
- Nuclear warfare
- Exploratory drilling (accidental breaching of the repository).

Many of these failures can be taken into account during the siting process; e.g., emplacement in deep, stable host rock. The chances of other failure mechanisms occurring can be reduced by good engineering design of surface and underground facilities and by control of the ground above the repository, e.g., preventing any drilling into the repository. In addition, the thermomechanical-hydrochemical breaching mechanisms remain. This study has only considered one or two hydrological breaching mechanisms.

Despite these limitations, which should be stated in the report, the analyses are valuable in that they discuss the type of hydrologic mechanisms that may be operating and provide for the relative comparison of two hydrological breaching mechanisms.

Regarding the granite simulations, the values appear to be excessively conservative for the following reasons:

a. The high values of hydraulic conductivity used in the analysis; these are not representative of values in a granite repository after site selection and extensive field testing has taken place (see Table 3.1).

b. The assumption of a "perfect tracer" that does not decay and is not absorbed into the rock matrix is in conflict with the KBS study, in which measurements of redox potential and oxygen content were made and mineralogical-chemical reactions observed. It was shown that reducing conditions prevail in Swedish granites at depth and that the groundwater lacks the ability to dissolve and disperse actinides to any great extent.

c. The presence of heat in a granite repository will reduce flow rates in the vicinity of the repository to less than 20% of the flow in unheated rock mass (see for example, "Effects of Heating on Groundwater Flow though the Fracture System of a Nuclear Waste Repository," D.E. Maxwell, B.C. Trent, D.M. Ross-Brown, EPRI Report 1981). The effect of heat could be taken into account by performing a flow analysis, taking into account the heat effects, and feeding the resulting hydraulic conductivities into the transport analysis.

Numerically, hydraulic conductivities between $10^{-0.89}$ ft/day(0.13 m/sec) and $10^{-3.40}$ ft/day(3×10^{-4} m/sec) (at depths below 800 feet in cores 24-25) were used in the analysis. This contrasts with the measurements made in Sweden and quoted in the KBS Report Volume 1 ("Handling of Final Storage of Unprocessed Spent Nuclear Fuel."

The Swedish investigators found that "most of the groundwater flow takes place in the upper part of the granite rock mass (10-300 m) where hydraulic conductivities are often between 10^{-5} and 10^{-7} m/s." Hydraulic communication in this section is generally good, which gives rise to a continuous and flat water table. A smaller portion of the groundwater flows through the deeper part of the bedrock, where its movement, for the most part, is restricted to certain water bearing zones. Intervening sections of rock have a conductivity of less than 10^{-9} m/s. Values of 2×10^{-12} m/s or less are quoted for the granite at Karlshamn, and 5×10^{-11} m/s for the granite at Stripa. In addition, the hydraulic connection between the individual fractures at great depths appears to be greatly limited.

TABLE 3.1 COMPARISONS BETWEEN DIFFERENT GRANITE STUDIES

Data Used	CGS (1)	DEIS (2)	KBS (3)
Depth of Repository	1100-1300 ft.	2000 ft.	1640 ft.
Permeability - good granite	$10^{-3.4}$ ft./day	1.4×10^{-6} ft./day	2.8×10^{-6} ft./day
Permeability - design values	$10^{-0.89}$ to $10^{-2.59}$ ft./day	1.4×10^{-5} ft./day	2.8×10^{-4} ft./day
Effective Porosity	0.0001	0.0001	0.001
Flow Rate			0.2 l/m^2 per year
Storage Coefficient		10^{-5}	
Hydraulic Gradient	0.034 (170'/mile)	0.001 (5'/mile)	
Results			
Flow time of host unit	10 days - 30 years	500 years	3,000 - 100,000 years

NOTES:

(1) CGS, Inc.

(2) Draft Environmental Impact Statement - assumed a loading of 100 kW/acre.

(3) KÄRN - BRÄNSLE - SÄKERHE, Report Volume 1.

(4) None of the studies allowed for crack closing due to thermal expansion of the rock, radioactive decay or cation exchange - factors which all tend to increase the escape time.

The Swedish data, based on 1500 conductivity determinations in granite masses, are the best data available. As far as is known, equivalent work has not been published in the U.S., although experiments are being conducted at the Colorado School of Mines Test facility. Since a U.S. repository in granite is expected to be located below 500 m, i.e., in the deep zone, using hydraulic conductivities between 10^{-8} m/s (2.8×10^{-4} ft/day) for transmissive zones and 10^{-10} m/s (2.8×10^{-6} ft/day) or less for non-transmissive zones should be used. The use of these values in the analysis may have a qualitative, as well as quantitative effect on the results.

As a result of these and other conservative assumptions, the authors predict that the time to initial contaminant breakout may be as little as ten days or as much as thirty years. This is surprisingly short for competent granite at depth, the type that would be considered as a host for a waste repository. The KBS results, based on extensive field testing of Swedish granites, indicated that the flow time from the peripheral parts of the repository to the surface may be more than 3,000 years at Finnsjö Lake. In the "good" granite at Karlshamn the flow time is "probably hundreds of thousands of years." In addition, the reducing conditions of the groundwater, the radioactive decay of the waste and the ion exchange capabilities of the rock mass act further to increase these calculated flow times.

Unfortunately, the KBS data base and study were not available to the authors during their study. Whatever data base is used, there is a need to carefully review the data, preferably by an independent panel of experts. The calculations should be repeated using more realistic input data.

The concentration distribution for different cases shown in Figures 2.4, etc., seems strange. As stated in the report, decay is not considered; therefore, material cannot appear and then disappear with time. It would be worthwhile to check the material balance at various times to see whether the total mass of nuclides is conserved.

While the concept of using the flow field as a first approximation to the nuclide migration is good, it does not appear that nuclides having strong ion exchange retardation can be accounted for in the probabilistic term. The text indicates that retardation is accounted for by changing the size of the reference particle. It is not clear how this changes the velocity, although it would change the quantity of material undergoing migration.
The verification of the deterministic-probabilistic method was so good as to be questionable; however, the reader does not have access to the information on the input/output to the various models to verify the results independently. It seems that only hydraulic head values were compared for validation purposes. It is important to compare concentration distribution as a function of time between numerical models or with the analytical solution. If the concentration of a nuclide at a specified point in the porous media and at a specified time matches with results obtained from different models using the same site and the same input data, then it might be considered a good validation. Comparing hydraulic heads and obtaining an acceptable match only indicates that the fluid flow portion of the model being tested is valid. What about the nuclide transport portion?

3.2.5.1.3 Scope

The work as presented, is limited to the analysis of ideal particles. There is no treatment of ion-exchange retardation for a particular species nor of radioactive change of the species. The conductivities used in the study appear to be high. This may result in invalid conclusions.

The method of computing the hydraulic head has not been made clear. Apparently, it is through the use of Darcy's equation (1.3); however, this does not include the gravitational potential which varies from about 6,000 feet to 1,000 feet over the site. This encompasses the range of the hydraulic heads. It seems strange that the head equipotentials are often vertical in a homogeneous strata instead of showing gravitational effects.

The boundary conditions applied to Darcy's equation and to the convection equation are as follows: no flow boundaries on the left, right, bottom and part of the top. Such boundary conditions do not reflect the strata. In particular, it seems that flow through the right hand boundary would be expected since it is a continuation of sandstone of rather high conductivity.

The treatment of sources is not made clear nor are they shown to be obtained from water table flows.

3.2.5.1.4 Verification

Since the calculation pertains to ideal particles (no chemical species retardation and no decay), it can hardly be expected that all aspects of the code have been tested and verified, nor has a realistic geometry been used. The comparisons with SWIFT and analytic solutions, have shown that DPCT is correct at least to a limited extent.

Comparison with the Swedish results would go far in establishing the credibility of the code.

3.2.5.1.5 Presentation

None of the reports being reviewed provide a master plan which shows how they fit into an integrated program, nor how they fit into the industry-wide state of the art. We feel that this is needed.

This report does not make clear how the model should actually be applied to a realistic site-specific situation.

The report is also deficient in minor areas; e.g., not defining the units of concentration, not defining the meaning of percent release, and the use of logarithmic time ratios when the fraction would have more meaning to the casual reader.

3.2.5.1.6 Report Conclusions

The observation that a poorly conducting intrusion may serve to dam the flow should be further explored. How common is such an intrusion? Is this conclusion valid in three dimensions?

3.2.5.2 Report Compared with Criteria

3.2.5.2.1 Model Realism

Although the code validation looks good, it is believed that the DPCT method has not been fully tested, particularly for decay chains and nuclides that are strongly retarded by ion exchange. It would appear that deficiencies in these areas would be conservative. Radionuclide decay and growth could be introduced through the Bateman equation if it is assumed that all changes take place in the repository. It appears that the method might be difficult to use for transformations in transit. The velocity retardation could be accounted for by using a retarded flow field calculation for those chemical species so retarded. Again, it would be difficult to account for changes in chemical species in transit.

3.2.5.2.2 Methodology Validity

The methodology is valid subject to the remarks in Section 3.2.5.1.

3.2.5.2.3 Data Validity

The data are consistent with Campbell et. al. (4); however, these data are expected to produce conservative results. There is no uncertainty analysis.

3.2.5.2.4 Time Period Appropriateness

The time period is not specifically stated, but there appears to be no restriction in this regard.

3.2.5.2.5 Event Sequence Completeness

No attempt is made to use a complete set of event sequences in the analysis. The scenario selection was apparently made to demonstrate the methodology. Refer to Section 3.2.5.2.9 for a comparison of these sequences with that of the much more complete set of Campbell et. al. (4). Scenarios which have been omitted include: water impoundment near or over the site, intrusion, geologic change and well scenario.

3.2.5.2.6 Key Parameter Identification

There is no effort at key parameter identification.

3.2.5.2.7 Uncertainty Analysis

There is no uncertainty analysis.

3.2.5.2.8 Application of the Model for Licensing

A code like DPCT which also treats nuclide decay and ion exchange retardation could be used to model the release rate from a repository and hence address a central licensing issue.

3.2.5.2.9 Scenario Correlation between Sandia and CGS.

The CGS geologic model in bedded salt (NUREG/CR-1608, Report 5; Figure 2.1 shown here as Figure 3-3) is quite similar to the model used in Campbell et. al. (NUREG/CR-0458; Figures 1.2.2 and 3.3.3 shown here as Figures 3-4 and 3-5). The differences are in the shape of the shale-sandstone front end in Figure 3-3 occurring in the 25,000-50,000 ft. horizontal distance region. Figure 3-4 shows this region as shale with a lower stratum of sandstone. The Sandia work shows a sand and gravel and upper shale cap while the CGS model assumes a no-flow zone. The CGS model shows no lower river, however, and seems to treat a release from the host rock as a release to the environment. The way CGS treats this is somewhat confusing. Paragraph 3 page 9 of Report 5, states that the sides and bottom are

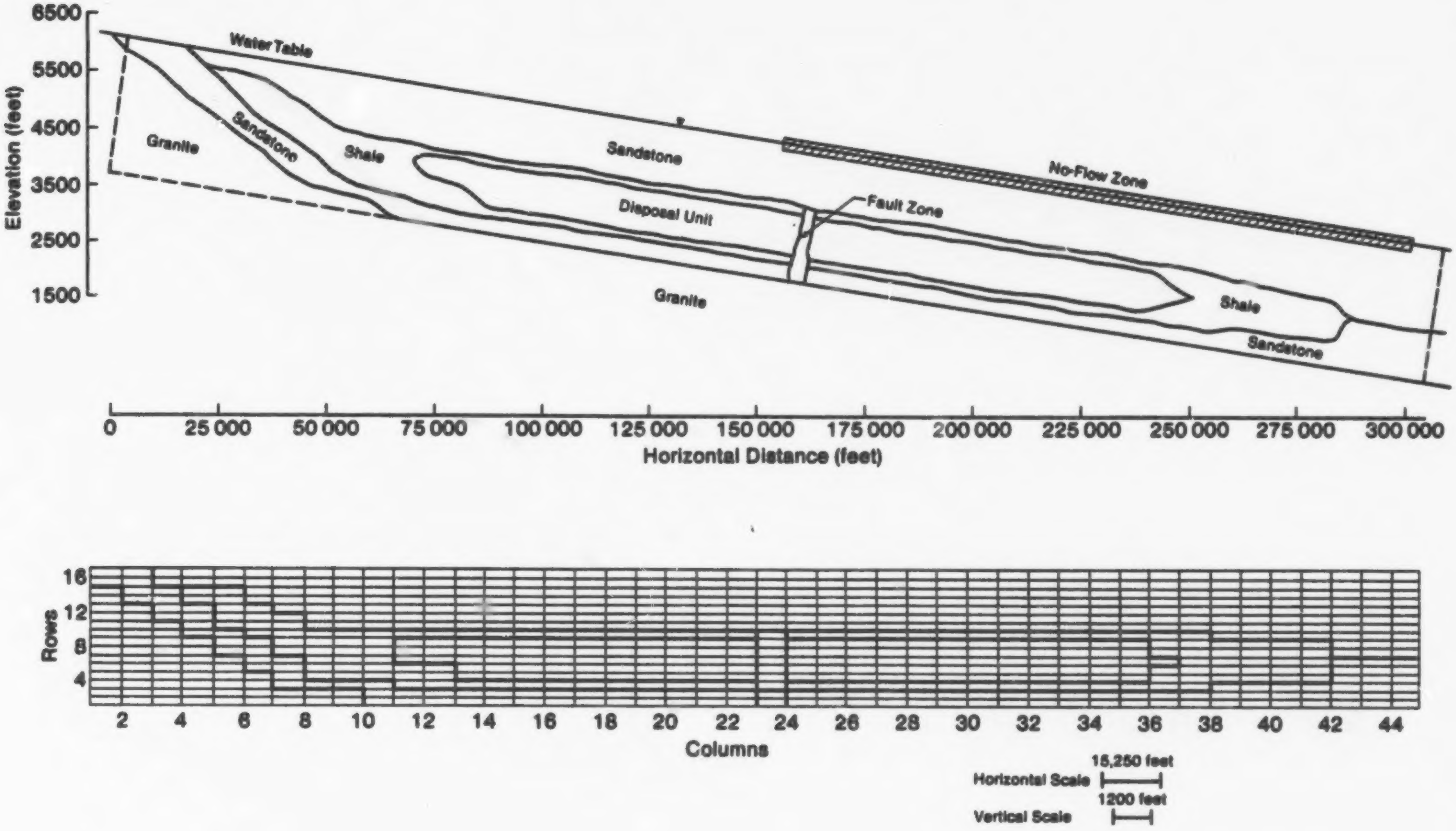


Figure 3-3. Geology and Model Grid for RRS in Bedded Salt.

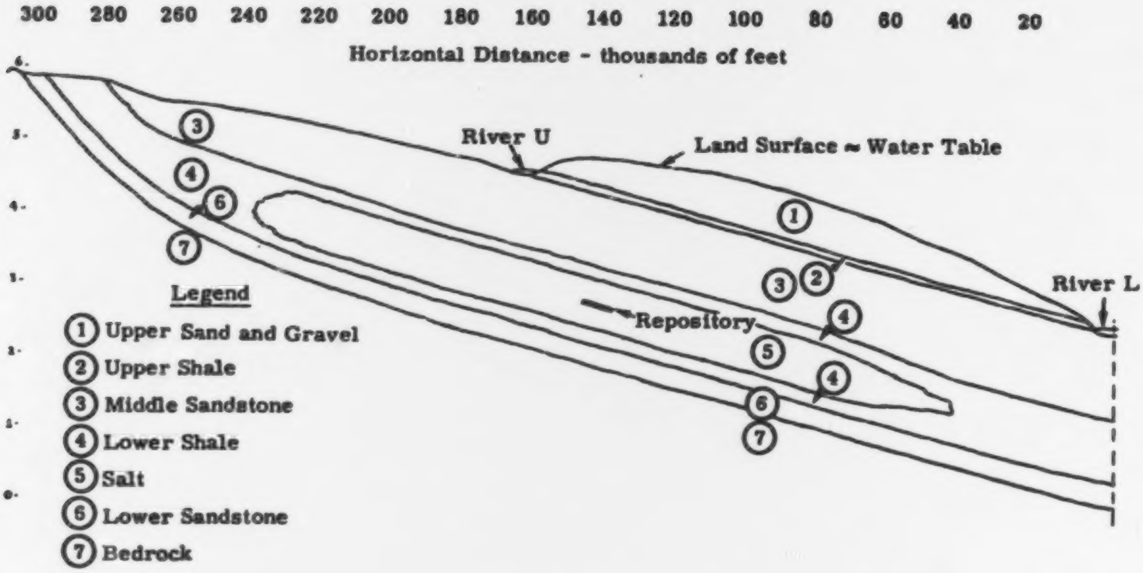
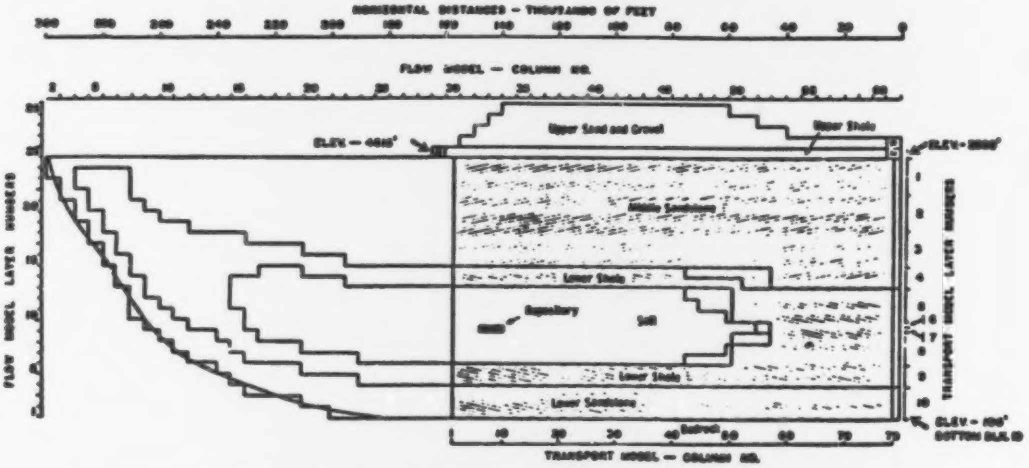


Figure 3-4. Geologic Cross Section at Reference Site (Vertical Exaggeration X20).



Right edge of Transport Col. 1 = Center of Flow Col. 30 = 187,000 ft.
Center of Transport Col. 79 = Center of Flow Col. 61 = 2,500 ft.

R — RIVER

Figure 3-5. Reference Site as Gridded for Transport Calculations.

no-flow boundaries. Figure 3-3 shows that half of the upper boundary is a no-flow boundary. The same paragraph states that ground water can only enter or leave through the upper boundary where heads are assigned. The Sandia scenario is understood to consider groundwater migration to the lower river which couples to the biota.

Referring to Report 5, Table A.1, the parameters that are presented, with the exception of the cation exchange capacity, also appear in Table 3.3.1 of Campbell et. al. (NUREG/CR-0458). The values of hydraulic and vertical hydraulic conductivity are the same in both tables, as are the porosity values. The longitudinal dispersion in Report 5 is 100 times smaller than the horizontal dispersivity in Campbell et. al. Campbell et. al. only give a value for lower shale; Report 5 uses the same value (5 ft.) for all rock. The cation exchange capacity (CEC) used in Report 5 is not realistic because it is the same for all rock and presumably for all chemical species. The value 0.1 is perhaps a nominal value; however, it is likely to vary with the type of rock and chemical species. No values are found for the CEC or retardation velocity in Campbell et. al.; however, the absorption distribution constant, K_{di}, is used in the equations on page 164.

CGS provides a model for a repository in granite that does not appear in the Sandia reports that have been reviewed to date; hence, no comparisons can be made.

The scenarios used by Sandia are different from those used by CGS. As stated above, Sandia uses a salt bed as a repository, whereas CGS uses both a salt bed and a granite bed. Table 3.2 provides a comparison of the scenarios considered by Sandia and CGS in salt bed repositories.

Table 3.2

COMPARISON OF SCENARIOS USED BY CGS AND SANDIA FOR SALT BED REPOSITORIES

SANDIA	CGS
(Scenario 1)	(Scenario A)
A U-tube connecting the depository to the overlying aquifer with radionuclide discharge at river L	No vertical disruption
(Scenario 2)	(Scenario B)*+
A U-tube to the overlying aquifer with radionuclide discharge at a nearby well	Vertical disruption in the downstream part of the system
(Scenario 3)	(Scenario C)*
A hydraulic connection between the overlying and underlying aquifers passing through the repository with discharge at river L	Vertical disruption in the central part of the system
	(Scenario D)*
	Vertical disruption in the upstream part of the system

---

*In each of the B, C, and D Scenarios, separate cases describe the impact of a vertical disruption of either high or low permeability with the repository (i.e., source) locations in the disruptive zone and downstream or upstream from the disruptive zone.

+Scenario B was also evaluated in a set of trials for a vertical disruptive zone with decreasing hydraulic conductivity from low to lower and lowest.

[redacted]

As seen from this table, the scenarios considered by CGS basically examine the consequences of disruptive features within a geologic repository system by assuming a high or low permeability fault zone. The scenarios considered by Sandia involve seal failures of a shaft on the up side or of a borehole on the down side of the repository.

The models used by Sandia or CGS are similar insofar as both are based on material balance and convective flow; however, the physical principles are somewhat different. The Sandia model considers retardation factors for nuclide transport, whereas the CGS model refers to ion-exchange between the radioactive species and the porous media. The leaching mechanism in the two models is also different. Although many terms are built into the CGS model, the simulation which has actually been used involves the transport of what the authors call a "perfect tracer". Such a tracer neither decays radioactively nor interacts with the porous medium. The models used by Sandia, i.e., SWIFT or NWFT, seem to be more complex than the CGS model. The Sandia models are not based upon as many simplifying assumptions. However, the emphasis in the Sandia work is placed on sensitivity analysis. Neither Sandia nor CGS have discussed how the results of their models can be verified or even whether the assumptions made on the governing physics are correct. It is realized that validation and verification of such models are very ambitious objectives; however, it must be done sooner or later.

Regarding the scenario criteria used by each party, - neither party states its criteria explicitly. The scenarios which have been most extensively developed seem to have been used in association with the nuclide transport calculation. Also, the scenarios seem to be based on readily found geologic conditions; the geology is not selected with the purpose of preventing a ground water release of the radionuclides. On the contrary, it would appear that the scenarios are contrived in the sense that the repositories are always forced to fail, possibly for the reason that if failure does not occur, the code is not extensively exercised. It appears that waste repository studies, in general, do not present explicit criteria for scenario development. In other words, this omission is not confined to the Sandia and the CGS work.

No attempt has been made to locate repositories in unusual geologic formations that would tend to prevent groundwater radionuclide transport. Perhaps an exception is the bedded salt repository, chosen because the presence of bedded salt is taken as evidence of the absence of groundwater movement over a long time. A weakness lies in assuming that after the geologic formation has been disturbed during the construction of the repository, the history of the formation will continue as before.

In the particular case of the Sandia/CGS scenario, it seems that placing the repository on a 2% gradient between two river systems is contriving a scenario for repository failure.

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APPENDICES

Line-By-Line Comments by Individual Reviewers

The specific comments entered in these appendices represent the questions or observations of individual reviewers as expressed in their monthly reports to the project manager. They are not necessarily consistent and some may not even be correct. However, they are probably representative of comments which other expert readers would have made when carefully reading the documents in their present form.

APPENDIX A

DOCUMENT 1

"...A Distribution-Free Approach to Inducing Rank Correlation Among Input Variables for Simulation Studies"

Page 3 Para. 1. Presumably "logit-normal" is a typo.

Page 3 Para. 2. The properties claimed for this method seem very worthwhile. Unfortunately, the absence of an overall scheme document for the Sandia work makes conceptualization difficult.

Page 4 Para. 3. It would be instructive to the reader if the authors provided an example or basis for the importance of the rank correlation coefficients to the repository modeling.

Page 4 Para. 3. The authors show good writing style in providing these linking paragraphs.

Page 4 Para. 3. This paragraph seems to suggest that by matrix manipulation of the definitions of X and C, the statement that XP' has the desired correlation matrix can be shown. I have not been able to achieve this result and do not believe it follows this simply. As a reader, I must accept the statement that "XP; has (is?) the desired correlation matrix C". What does one do with P' once it is obtained? Where does X come from, since it is stated that the elements of X are uncorrelated but the basic problem is that the input variables are correlated?

Page 5. The numerical example is good, however, one would like to see what the problem is which is being solved.

Page 6. Where does the C matrix come from? How is it related to nuclide migration or some other aspect of repository failure?

Matrix R is generated using algorithm C which uses a random number generator. From experience with random number generators, this one does not pass all the tests which show the degree of randomness. For example, it would not pass the so called "Poker" Test. Rows 3, 13 and 14 contains "three of a kind", three 5's in row 3, three 11's in row 13 and three 10's in row 14. There are several "two of a kind". It may not be essential to have very random numbers in matrix R, but if it is, then a better random number generator should be chosen.

Page 7. It would help if the authors described how the rank correlation matrix of R which is T was obtained. They have given the algorithms A, B and C in the Appendix, maybe they could show how matrix T is derived knowing matrix R.

Page 9. The various matrices of numbers seem quite abstract since the reader does not know how they relate to the calculation of repository risk.

Page 10 Para. 2. "The rank correlation matrix L...does not turn out to be exactly equal to C". This seems a gross understatement. The two matrices are equal on the diagonal but in few other elements.

Page 11. Table 1 is a very good demonstration of effect of sample size on reducing the error. Comparing the numbers for x in sample sizes 15, 25, 50 and 100 in Table 1 for i, j of (4,5), (4,6) and (5,6) it seems that the value -.6766 corresponding to (i,j) of (4,6) and N=25 is inconsistent. Is it possible that the number was -.6796 and the error may be typographical?

Page 12 Para. 1. This application omits so many of the physical details that it can hardly be called an "Application". For example, what are the 15 variables used in the example? How do you know the variable correlations in the absence of the physical process to which the variables relate?

What is meant by "Target Correlation Matrix"?

Page 15 Para. 2. This paragraph seems an excellent statement of the aim of this report. It could be expanded upon and placed earlier in the report.

Page 20. In line 2 from the top there is a misprint "trangular" instead of "triangular".

In algorithm C, the Dimension ID (1) the number inside the parentheses must be greater than 1, possibly N.

APPENDIX B

DOCUMENT 2 -

"...The Distributed Velocity Method of Solving the Convective-Dispersion Equation."

Page 1 Para. 1. "...in the context of a risk analysis methodology." Throughout the Sandia work the meaning of risk is vague. Presumably it has something to do with the probability of harm although it could be harm without any probability consideration. The sentence, "Furthermore, radionuclide migration times from the depository to the surface environment are typically long so that radionuclides in the actinide chains are likely to be significant contributors to risk." is quite oblique. The authors are stating that from a priori knowledge the migration times are typically long; therefore only long-lived radionuclides are apt to survive long enough to reach the surface. Some actinides are long-lived and have a large biological effectiveness because of the way they enter the food chain and are retained in the body, hence actinides are likely to be significant risk contributors.

Page 13. In the nomenclature is defined as concentration. In the text, it is referred to as density. There is a clear distinction between the two. Consistency would help the reader.

Page 13 Para. 3. P(v) must be a distribution density for dimensional correctness (see Equation 2-1).

Page 13. On the last line, instead of "...at time t' ", it should be "...at time t."

Page 13-14. The model as presented needs interpreting. It is visualized that particles at x',t' travel to x,t with a velocity distribution density P(v). Since v = (x-x')/(t-t'), if x, x', t and t' are all specified v also is specified and hence its distribution is a delta function. Therefore in Equation 2-1 the variables are v and t' with t' given as

$$t' = \frac{x' - x + vt}{v}$$

and the equation is $\rho_0(x,x',t) = \int_{-\infty}^{\infty} dv\ P(v)\ \rho(x',t')$

or

$$\rho_0(x,x',t) = \int_{-\infty}^{\infty} dv\ P(v)\ \rho(x', \frac{x'-x+vt}{v})$$

which is only a more explicit form of Equation 2-1.

Equation 2-3 does not seem to be correct for the reason just stated, namely that the relationship $x' = x-v(t-\tau)$ imposes a constraint on the variables and it is not possible to integrate over x' and v independently. It would seem that the injection source would have the same form as the original source and they should be combined by superposition.

Page 14. The author should define what τ is in the text and give a better description of the source term S.

Page 16. The author seems to distinguish between $\bar{v}$ (average velocity) and Equation (2-13) which is a definition of average velocity. It would help if the definition of $\bar{v}$ is better clarified.

Page 16. In Equation (2-11), a velocity v appears which has not been previously defined. It should be $\bar{v}$.

Page 16. Equation 2-11 can be understood only if it is

$$G(x-x',\ t-t'] = \frac{1}{\sqrt{2\pi}\ \sigma_x} \exp - \left\{ \frac{[(x-x') - \bar{v}(t-t')]^2}{2\ \sigma_x^2} \right\}$$

where the original v is changed to $\bar{v}$ which is presumably the mean value of the velocity distribution.

Now if $\sigma_x^2 = 2D(t - t')$

and $v = (x-x')/(t-t')$

then by substituting 2-12 and 2-13 into 2-11 it is found that

$$G(x-x',t-t') = \frac{1}{\sqrt{2\pi}\ \sqrt{2D(t-t')}} \exp\left\{ \frac{[v(t-t') - \bar{v}(t-t')]^2}{2 \cdot 2D(t-t')} \right\}$$

$$G(v,t-t') = \frac{1}{\sqrt{2\pi}\ \sigma_v(t-t')} \exp\left\{ \frac{(v-\bar{v})^2}{2\sigma_v^2} \right\}$$

where $\sigma_v^2 = 2D/(t - t')$

Note that the function t defined in Equation (2-15) on page 18 contains a typographic error. The exponent

$$\left\{ - \frac{(v - \bar{v})}{2\ \sigma_v^2} \right\}^2 \text{ should be } \frac{-(v - \bar{v})^2}{2\ \sigma_v^2}\text{, as indicated above.}$$

Also, at the bottom of the page there is a reference to Equation (2-2), but there is no such equation in the report.

Page 19 Para. 2. "The velocity dimension is divided into N_v increments based on equal probability." Equal probability of what? Velocity? Particle density?

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Page 19. In the sentence, "The velocity dimension is divided into N_v increments based on equal probability.", there appears for the first time the concept of probability. The writer should make clear what he means by "probability" in this context. Is he referring to equal areas, or what?

Page 21. The author admits that his choice of notation for indicating the spatial variation makes understanding of Equation (3-1) a formidable task. It is suggested that single letter subscripts be used rather than the letter subscripts. For example let i = receiving block, k = donor block, then,

x_{i-1}, x_i, x_{i+1}	will indicate the blocks after block i (receiver)
x_{k-1}, x_k, x_{k+1}	will indicate the block k (donor)

Page 21. Is there a V missing from the left hand side of Equation (3-3)?

Page 21 Eq. 3-3. The meaning of this equation is not obvious. Apparently one specifies j, σ_v and N_v then v_j is that velocity having a probability of $(j-1/2)/N_v$, but to what purpose?

Page 22 Eq. 3-7. If this equation is the new solution, what happened to the diffusion coefficient? Is it somehow contained in the velocity distribution?

Page 26, General Comment. One reviewer found the description of the numerical methods, which also represent an extension of the theory, to be very opaque. It is felt that either steps are left out or poorly explained. In either case confidence in the results is not enhanced.

Page 27. What is meant by "leached but undissolved"?

Page 27. The formulation and description on the source and discharge models are handled very well. However, I do not agree with the way the author has divided the radionuclide inventories in the source model. In accordance to chemical engineering definitions, there is no way to have leached but undissolved (category (2) given by the author). I would suggest dividing the source radionuclide inventories as follows: (1) unleached and undissolved, (2) leached but not dissolutioned (no chemical reaction), and (3) dissolutioned.

Page 27 Eq.3-16. One would think that the leach rate is proportional to the surface areas. Also m_0 is time dependent due to decay.

Page 29 Eq.3-20. The use of MIN is assumed to mean that the nuclide density does not exceed the solubility limits.

Page 30, General Comment. It would be interesting to know if the DVM method presented satisfies the conservation of mass and flow constraints used in the SWIFT model.

Page 32. (1) It is suggested that the authors describe the boundary conditions in Eq. (4-2) and Eq. (4-3) in words as well as in Equation form.

(2) There is a ρ missing from left hand sides of Eqs. (4-2) and (4-3) i.e., Eq. (4-2) should be $\rho(x=0, t) = 1$.

(3) It should be mentioned that the source term is dropped when trying to obtain Eq. (4-4) from Eq. (2-8).

Page 35 Para. 1. Why were points sampled from a loguniform distribution?

Page 37 Eq.4-6. It is not obvious to the reader that the second term is negligible since D (or α) is not given. In fact the positive exponential could be quite strong.

Page 39. In restating Eq. (4-13) to arrive at (4-15) it seems that 0.859 should be 0.859×10^{-5} L. Eq. (4-15) should be checked.

Pages 40-41. Figures 4a - 4d all are titled "Effective Dispersivity for Several Values of Peclet Number." It is suggested that the following be used:

Figure 4a. Effective Dispersivity for Peclet Number = 1
Figure 4b. Effective Dispersivity for Peclet Number = 5
Figure 4c. Effective Dispersivity for Peclet Number = 10
Figure 4d. Effective Dispersivity for Peclet Number = 100

Page 42. Same comment as Page 39. Eq. (4-19) needs checking. It seems that 0.859 should be 0.859×10^{-5} L.

Pages 44-45. Same suggestion as pages 40-41. Figures 5a - 5d should be retitled to state the value of the Courant number corresponding to each figure.

Page 50. In comparing the analytical and numerical solutions with DVM (Figs. 6, 7, 8) it would be interesting to see the effect of Peclet numbers and Courant numbers when ΔX and Δt are kept constant and other parameters are varied to obtain different values for P and C and compare the analytical with DVM. This will mean changing the initial parameters of the problem but it should provide an interesting comparison.

Page 51 Para. 1. Why didn't the authors compare their results with TASC's one-dimensional Green's function code?

Page 51 Para. 1. The authors ask the question "Why should one use DVM?", but they do not answer the question in the remainder of this section.

Page 53 Line 9. The author states that "it is clear from Figure 5b...the numerical dispersion could be further reduced by increasing the time step." This is not clear at all. Figure 5b gives α_{eff}. vs. α for C=1. Since $C = \frac{V\Delta t}{\Delta x}$, C=1 implies $V\Delta t = \Delta x$. Hence at constant V, as Δt increases Δx must also increase to keep C=1.

Figure 5b shows that α_{eff}/α for any α becomes larger as Δx increases. Therefore, an opposite result than that suggested by the author is obtained. Some clarification is required.

Pages 57-58. Both Figures 10 and 11 show perfect matches of DVM with the analytical and FD. I wonder how much of it is due to choice of the time scale. I would suggest use of an expanded time scale for A and C. Rather than showing DVM with a line and the others with points it would be better to show all of them with different lines. If perfect matches are obtained it may help to give tabular comparisons rather than graphical.

Page 59 Para. 1. DVM does not seem new if viewed as a Green's function solution of the one-dimensional transport problem.

Page 59 Para. 3. The authors do not demonstrate the computational efficiency of the method in set up time or memory. In fact, the reader is left with the feeling that this is one of many solutions without the advantage being presented.

It is suggested that further testing be performed before generalizations are made regarding the effect of time step size or accuracy. For example, test the technique using constant V and ΔX and only change Δt to arrive at different Courant numbers. Start out with C = 0.5, increase Δt to get C = 5, and keep increasing Δt until the limit is reached, i.e., the breakthrough is reached in one time step.

Page 60. Better results are obtained with shorter computer time (larger time step size); this doesn't seem likely. The reasons for this unique advantage of the DVM method should be given and explained.

Typographical Errors

Page 13.	4 lines from bottom, first word - and should be "an"
Page 22.	Eq. (3-8) k_j-1 should be k_{j-1}
Page 27.	7th line from bottom and and (3) should be and (3)
Page 36.	Table 1. It seems that α is missing from list of variables
Page 53.	Lines 8 and 9 - 5B should be 5b
Page 54.	Table 3. x should be Δx t should be Δt

APPENDIX C

DOCUMENT 3-

"...Transport Model Sensitivity Analysis"

Page 5-6. The abstract is misleading. It implies that sensitivity calculations were performed with SWIFT. This is true only to the extent that sensitivity studies were performed to conclude that NWFT results were satisfactory. SWIFT was used to provide the flow field input to NWFT but the sensitivity studies were performed using NWFT.

Page 9 Para. 1. Risk analysis consists of two parts: probability and consequences. The list of items presented only relate to the consequences.

The paragraph mentions large uncertainties in the point estimate of risk; yet how does this report, or the sensitivity procedures in general, address uncertainty? It seems that some of the mathematical machinery is not useful if the end result is to provide confidence bounds.

Point estimates of the risk are not meaningless, provided the basis for the results are known; they may be misleading if the uncertainty bands are large or they are not considered in their statistical context, i.e., long-term averages.

Page 11 Para. 1. It doesn't seem that the important parameter is the time at which groundwater contacts the radioactive waste but rather the time at which the wastes begin to be transported by the groundwater. Possibly this is what the authors mean but some people think of the waste as consisting of the radionuclides in a matrix inside of a canister.

Page 11 Para. 2. Some people believe that only the engineered barrier can be depended upon, i.e., the barrier consisting of the waste matrix and canister. It is not clear how the sensitivity methods presented here would apply to the analysis of this barrier.

Page 12 Para. 4. "The first is to ascertain which variables have a statistically significant effect upon total discharge." This sentence is a little confusing. It seems that there is a deterministic relationship between a variable and the discharge as far as the modeling in this report.

Page 12 Para. 4. "...at the 5 percent level." Do the authors mean that for the full range of uncertainties in Table 5, the effect on the discharge is 5 percent or more? If so, this is a very weak coupling.

Page 12 Para. 4. How does the method address distribution assumptions? It uses the distributions in its sampling procedure but does not generate distribution of the output for the input distributions.

Page 17. Forty inches of rainfall per year is quite high. Why would anyone consider building repositories in such areas?

Page 18. It would help to show the line of symmetry. Perhaps that is the wiggly line at the bottom. Presumably the repository location as shown is the surface facility. Do the X's show the cut for Figure 3?

Page 19. In Figure 3, "Vertical Exaggeration x 20" cannot be correct. Why doesn't Figure 3 have a vertical scale?

Page 20. Gas and oil companies have looked at salt domes as possible storage space for years. They must have geological and hydrological data on salt deposits.

Page 22. Figure 5, does the size of arrows have any significance as to the magnitude of the velocity vectors?

Page 23 Para. 1. Is any information available on the probability of these three scenarios? If not, it will be difficult to determine the results in terms of risk.

Page 23 Para. 2. Isn't three feet in diameter very large for a bored-hole?

Page 23 Para. 3. While it is agreed that the flow path in Figure 7 is possible, it seems that the code should be used to calculate the time to deform the depository to reach this state. The depository when closed will not have the path as shown and it will require a long time for groundwater to excavate the U-tube as shown. Of course, the purpose of this report is to do sensitivity studies, not to develop models; however, the time to achieve the scenario could greatly affect the time scales considered and thereby throw off the radioactive decay calculations.

Page 27. "Figure 8. U-Tube Formed Through Depository". I see no U-tube in the figures.

Page 30. I don't quite agree with the ranges picked for the variables in Table 1. For example, what is the significance of α varying from 45-500 feet? Why 45 and not 50 or 100? Ranges for K_d of U, Th, and Ra are within 7 orders of magnitude. I am quite familiar with the uncertainty in the K_d data but only within 3 orders of magnitude and not 7. τ varies from 10^3 to 10^7 years, whereas total discharged is integrated over 10^6 years.

Page 30 Table 1. What is the basis for selecting the distribution of the variables? What is the meaning of the range of values and how do they relate to the distribution, i.e., can the range be used to obtain the parameters of the distribution?

Page 33 Para. 1. Is not using the same distribution coefficient for the shaft and aquifer essentially the same as postulating that an aquifer couples water to the waste canisters? This is an extremely pessimistic view of repository design and amounts to postulating engineering failure and just calculating the transport time.

Page 34 Para. 1. "...the response surface is not an important product of the analysis." If this is so, why the discussion of the response surface on pages 13 and 14? Is the whole purpose of this exercise to rank the variables in decreasing order of their effect on the maximum radionuclide release rate and on the total release? A response surface contains more information because with a response surface one can find the output variance reduction for certain input variable variance reductions and from this an error analysis can be constructed.

Page 34. "However, to provide confidence...original SWIFT output." How about a simple test as follows: A base case can be formulated by choosing the most probable input variables. The cumulative discharge can be calculated using the base case inputs. The importance of one variable versus another can then be obtained by comparing the variation caused in the total discharge against the variation in the different variables over their particular range.

Page 35 Fig. 10. The figure states that "All discharge results are normalized to the maximum observed discharge." Does this mean that both NWFT and SWIFT were forced to agree on the maximum discharge values or that each are separately normalized to their peak?

Is NWFT able to absolutely reproduce SWIFT calculations or is it useful only in a relative sense after being normalized to SWIFT.

A second point about the figure is that the cumulative relative frequency estimate should be explained. We interpret that this is the cumulative relative frequency of observing a discharge value for each Latin hypercube sampling of the input variables.

Pages 37-41. The technique outlined on this page to compare SWIFT and NWFT models does not seem to be fair. I am sure that a different procedure could be set up to show that SWIFT is better and vice versa. The authors' justification of using NWFT rather than SWIFT for the rest of the tests is not correct. They do admit that NWFT can only handle isotopes with equal K_d, yet K_d is one of the important input variables. In a multicomponent system both K_d and solubility are not only independent properties of individual isotopes but depend to a great extent on the presence of other nuclides. Sometimes the variations due to mixing (presence of other isotopes) can be greater than the magnitude of the property for the pure component.

Page 41 et. seq. Why is this theoretical development presented? It seems to have nothing to do with the sensitivity analysis of NWFT?

Page 42 Table 5. Why is the lower limit on the porosity different from that of Table 1?

Pages 44-47. I would only like to add that choosing D as a symbol for dispersion coefficient in Equation (1) and D as the rate of discharge in Equation (4) only adds to the confusion.

Page 45 Line 14. The equation:

$$G(t) = \text{erfc}\ \frac{z-vt}{\sqrt{4\alpha vt}} + e^{z/\alpha}\ \text{erfc}\ \frac{(z+vt)}{\sqrt{4\alpha vt}}$$

is incorrect. It can be corrected, however, by substituting the quantity $\frac{v}{R}$ wherever v appears.

The presentation of material in this report is somewhat confusing and could be improved. The rate of discharge is derived as

$$D(z,t) = \frac{I}{2\tau}\ e^{-\lambda t}\ [G(t) - G(t-\tau)\ S(t-\tau)] \quad ,$$

as is seen from Equations (2) and (4). Yet, this is never used. Instead, numerous graphical results for the total integrated discharge are presented, but no corresponding equations appear in the report. The dependence of the total integrated discharge on various parameters is explained and supported by lengthy discussion. In this context, it would have been useful to present an analytical representation for the total integrated discharge. This would have been more informative to the technical reader than the lengthy discussion, and it would have made the trends easier to understand. An analytical representation for the total integrated discharge (over all time) can be obtained as

$$D(z) = \int_0^\infty D(z,t)dt = \frac{I}{\lambda\ \tau} \left[1-e^{-\lambda\tau}\right] e^{-\frac{z}{2\alpha}\left[\sqrt{1+\frac{4\alpha\lambda R}{v}}-1\right]}.$$

Similarly, for the no dispersion case ($\alpha=0$), the following is obtained:

$$D(z) = \frac{I\ e^{-\frac{R\lambda z}{v}}}{\lambda\ \tau} \left(1 - e^{-\lambda\tau}\right).$$

Such results could provide the reader with additional insight regarding the dependence of the total discharge rate on the various parameters. Additionally, they can aid the user of the SWIFT or NWFT codes to verify that these codes are working properly, or they can serve as additional tools for the benchmarking of these codes.

Page 48. The theoretical development (Section 5.1) ends with definitions of leach rates and solubility limit and yet it does not show how the total discharge will be different for the leach rate limited and solubility limited cases.

Page 48 Para. 3. The results of Figures 14 through 17 seem meaningless in that the total discharge should increase as the half-life increases for any scenario. A scenario in which the total discharge decreases with increasing half-life has not been proposed.

Page 53 Para. 1. "The latter quantity (R^2) assumes values from zero to one which, when multiplied by 100, indicates the percent of variation in the total discharge which is explained by the accompanying variables." There is only a single value of R^2 given in Tables 7 and 8. One number cannot explain the variation caused by each of several variables. Perhaps the authors mean that of the variables listed (excluding squared terms of a variable) the percentage given is the variation caused by the set.

(Comment on the above remark: This remark indicates that the meaning of statistical terms such as total variation, explained variation, and the coefficient of determination, R^2, are not universally understood. Hence, a brief discussion of these terms would be beneficial.)

Page 53. Second paragraph: The sentence starting with "The selection....coefficient" does not make sense.

Page 53 Para. 3. $1/\tau$ is a leach rate not leach time as stated. The reason why larger leach times (smaller leach rate) should affect the long-lived isotopes more strongly than the short-lived ones is not apparent. One would think that the opposite is the case because a long leach time would result in the short-lived isotopes decaying in the canisters.

Page 55. In Table 8, the R^2 for half life of 10^6 years is 0.76. The authors claim that R^2 increases as half life increases. Should R^2 be 0.96 instead of 0.76 or is there some other explanation?

Page 56 Para. 2. What is the meaning of the "Rank Correlation Coefficient"? How do they numerically indicate the importance of the independent variables on the dependent variables?

Page 59. Figures 19-22 could be combined with Figures 14-17. It would save pages and also provide ready comparison between Leach-Limited Source and Solubility Limited Source. The same reasoning applies to combining Tables 7 and 8 with 9 and 10.

Pages 63 & 65. Unlike Tables 7 and 8, 9 and 10 do not show an increase in R^2 with respect to an increasing half life. There should be an explanation of why this does not happen.

Page 64 Para. 2. It should be noted that NWFT does not calculate the well water salinity hence it is not possible to judge the consumption of this contaminated water. One would expect it to be highly saline because of the ratio of solubility of salt to the radionuclides.

Pages 74-77 Figures 29-32. As stated before, the plots of cumulative frequency versus total discharge have little meaning. To illustrate, Figure 32 says that in 94% of the trials about 1/2 of the repository was released, if radionuclides have half-lives of 10^6 years. But Figure 31 says the same thing for half-lives of 10^5 years. These figures seem to say little about sensitivity. The sensitivity is contained in Table 12 presented as standardized regression coefficients.

Page 78. It is suggested that the authors compare Figures 19 to 22 with Figures 29 to 32. If the comparison is important, these figures should have been combined.

"Section VI. Results and Conclusions." It is stated that the geological and hydrological data used in the study are characteristic of real sites. It would be interesting to know which real sites had a porosity of 0.003 as given in Table 5. It seems that the range of input variables were chosen such that it could fit the universe of possible values. Results given in this report seem to indicate that the relative importance of an input variable depends on the magnitude of the range. Therefore, it is essential to choose realistic ranges.

Page 82. The second part of the third conclusion will be a function of how the problem was set up.

APPENDIX D

DOCUMENT 4

"...Small Sample Sensitivity Analysis Techniques for Computer Models with an Application to Risk Assessment"

Page ix. The authors talk about three *types* of models. It would be less confusing if the word *type* was replaced by *example*. Use of the word *type* may give the reader the impression that the authors are going to categorize models into distinct classes such as deterministic versus stochastic.

Page x. The authors make the following statement, "Extraction of the amount of information indicated in the previous paragraph requires the development of new statistical techniques."

It is not clear why new statistical techniques are needed. Their argument might have been more convincing had the authors presented a brief statement regarding why they believe existing statistical methods are inadequate.

A statement like, "Latin hypercube sampling, as introduced by McKay, Conover and Beckman (1979) appears to provide a satisfactory method for selecting input variables...", is rather vague. If one were considering the possibility of using Latin hypercube sampling, one would like to know whether or not the method is advantageous and the conditions under which it may be applied correctly, not that it *appears* to be satisfactory.

Page x. Reference is made to a report written by McKay, Conover and Whiteman (1976). This informal report (LA-NUREG-6526-MS, Los Alamos Scientific Laboratory) is not readily accessible. It would have been considerably more convenient had the authors listed references that are more accessible. Clear introductory discussions regarding partial correlation appear in many texts, e.g., Wonnacott & Wonnacott, *Econometrics*, Wiley 1970, pp. 127-129. Why not refer to such sources of information?

Page x-xi. The remainder of the executive summary is more a description of the organization of the report than a summary of the key ideas and conclusions.

The authors state on page xi, "Comparisons are also made among other sampling procedures such as replicated Latin hypercube sampling and random sampling." It would have been a lot more informative if the authors had presented a summary of their results.

The authors mention that their method (presumably they are talking about Latin hypercube sampling) is flexible enough to adapt to unusual situations that may develop. It is not clear exactly what they mean by flexible. Also, it is not exactly clear what they mean by unusual situations. In general, the authors fail to present a convincing argument (motivation) in support of their approach.

Page 1. The first sentence would be improved, to some extent, if the phrase "amost (sic) certainly involve" were replaced by "require."

Page 2 (bottom). As mentioned previously, the authors claim: (1) new statistical methods are required, and (2) Latin hypercube sampling (LHS) appears to provide a satisfactory method. These claims should be supported by specific examples and/or other convincing evidence.

Page 3 (top). Reference is made once again to the McKay, Conover and Whiteman (1976) report which, as previously stated, is not readily accessible. A number of authors have written good expository discussions regarding partial correlation coefficients. These appear in standard statistical texts so why not refer to these publications? If the McKay, Conover, Whiteman report contains something special, then why not present a summary of its contents?

Page 3. (10th line from top) Change "asumed" to "assumed."

Page 3. (3rd line from bottom) Change "...conditions would become..." to "...conditions will be...."

Page 4 Para. 2. The authors should use the term "risks" with great care. Several definitions of risk appear to have been accepted by the scientific community. The authors should make clear how their methodology relates to a specific definition of risk or method of risk assessment.

Page 6 (8th line from the top). The statement, "For codes in which the input variable is a monotonic function of one input variable, stratified sampling of the input variable usually results in a substantial decrease in the variance of the estimators...." is a rather vague statement. What do the authors mean by "usually results in a substantial decrease"? It would have been more informative had the authors indicated how substantial the decrease in variance may be, e.g., 10%, 50%, 75%? It has been stated that monotonicity is a sufficient condition. It would be nice to know whether or not the LHS method is robust. In other words, does the LHS method yield reasonably good results when the function is not monotonic? We realize that the authors are only providing the rationale behind the LHS method at this point; however, their discussion might have been considerably more convincing had they provided some supporting evidence at the outset.

Page 7 (8th line from bottom). The statement, "...it is reasonable to assume that the input-output relationship is monotone in most cases." should never have been made without supporting evidence. There is no reason to believe this statement is true unless the authors are implicitly assuming that the effects under investigation are cumulative effects, e.g., the integral of a function which is always positive or always negative. Also, it is not clear what the authors really mean when they say "in most cases". Such vague statements should be avoided.

Page 8 (bottom). The last sentence which reads, "The probability $p_{k,n}$ of each interval is defined as $p_{k,n}=P(X_k \in I_{k,n})$." should be changed to read: "The probability size, $p_{k,n}$, of each interval, $I_{k,n}$, $k=1,2,3,\ldots,K$; $n=1,2,3,\ldots,N$ is defined as $p_{k,n}=P(X_k \in I_{k,n})$."

[redacted]

Page 9 (4th line from top). The assumption of statistical independence between the input variables is an important assumption that should be made explicit, both at this point as well as in a list of all the key assumptions and limitations at the beginning of the report.

Page 9 (6th line from top). "$I_{1n_1} \times I_{2n_2} \times \ldots \times I_{kn_k} = S_{\underset{\sim}{n}}$ (2.4)". should be changed to read as follows:

$$\text{"}I_{1,n_1} \times I_{2,n_2} \times \ldots \times I_{k,n_k} = S_{\underset{\sim}{n}} \qquad (2.4)\text{".}$$

Also, (2.5) should be changed to read:

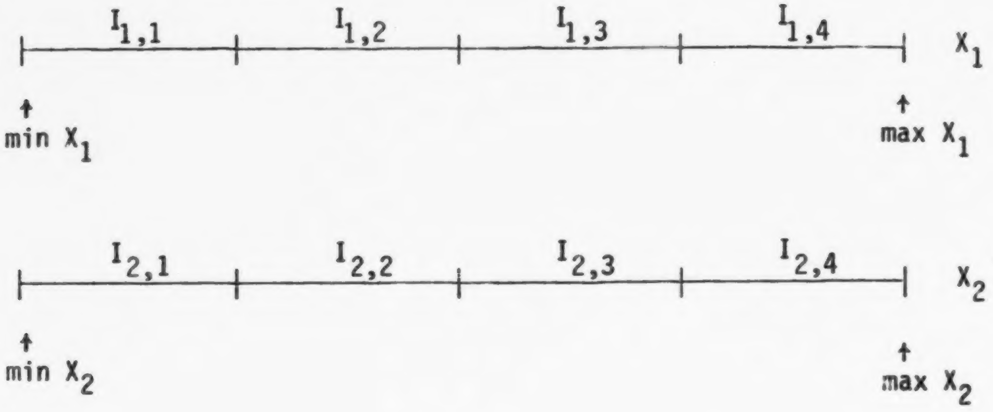
$$\text{"}P_{1,n_1} \bullet P_{2,n_2} \bullet \ldots \bullet P_{k,n_k} = P_{\underset{\sim}{n}} \qquad (2.5)\text{".}$$

Equation 2.5 should be preceded by a statement such as:

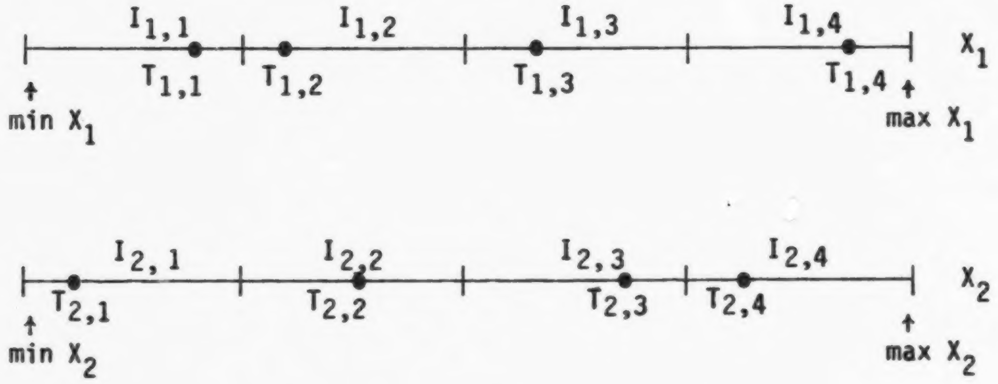
> "Under the assumption of statistical independence among the input variables, the product
>
> $P_{1,n_1} \bullet P_{2,n_2} \bullet \ldots \bullet P_{k,n_k} = P_{\underset{\sim}{n}}$
>
> represents the size of the cell denoted by the K-tuple $\underset{\sim}{n} = (n_1, n_2, \ldots, n_k)$, where n_j denotes the interval from which the value of X_j is drawn.

Page 10. The discussion of the LHS procedure is correct; however, there is much left to the reader's imagination. For example, when N is large, how are the random permutations actually generated? What are mutually independent permutations? How are "random observations" actually generated? A simple example would suffice. Consider for example, the case where N=4 and K=2. Four ordered pairs are to be generated. When carrying out the LHS method proceed as follows:

Step 1. Partition the domain of X_1 and the domain of X_2 into 4 overlapping intervals as shown below.

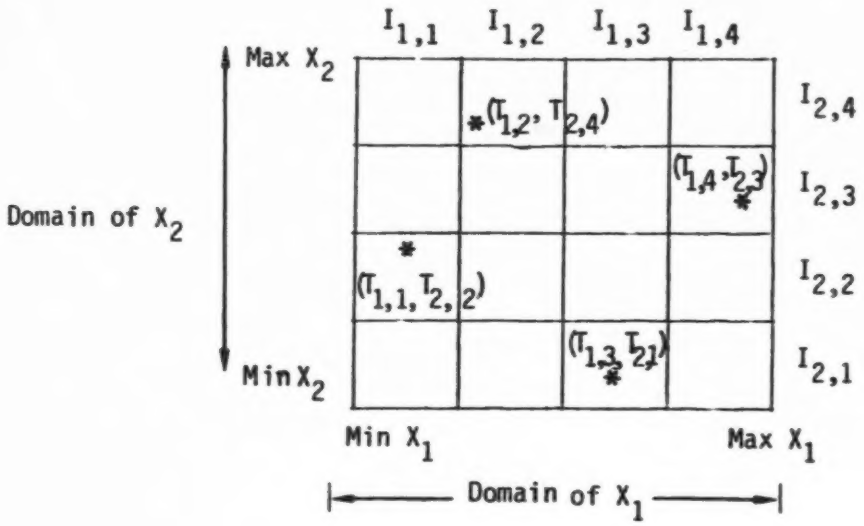


Step 2. Randomly draw a single value, say $T_{k,n}$, from each of the intervals $I_{k,n}$, for k=1,2, n=1,2,3,4.



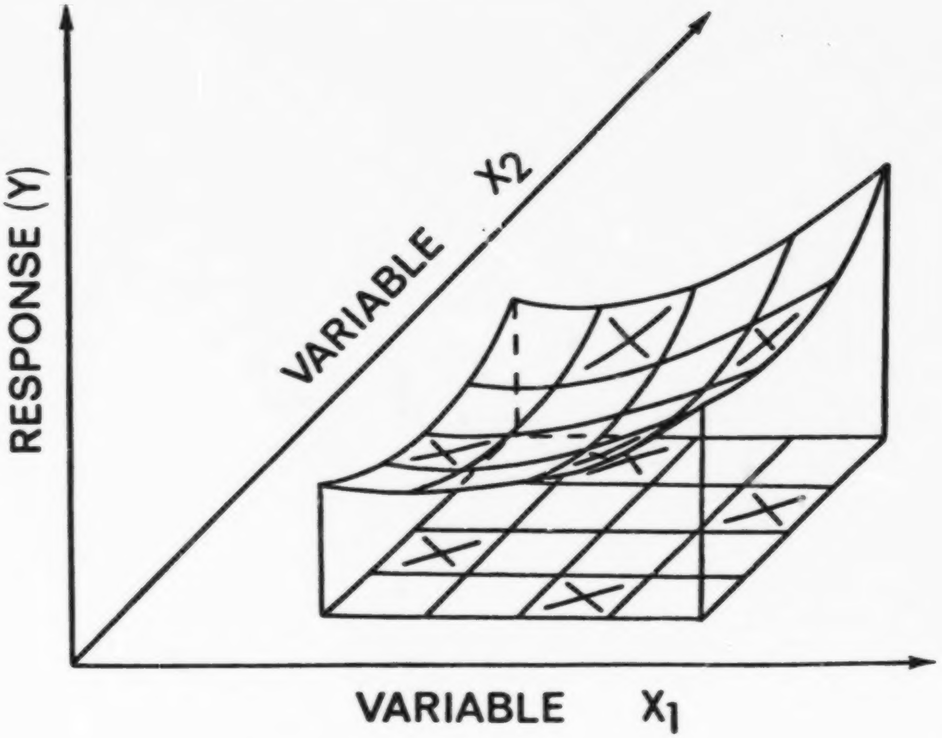
Note: The mechanics associated with the actual sampling scheme should be explained in an appendix. For example, for each interval, $I_{k,n}$, one may generate a single value of u, where u is uniformly distributed on (0,1). Then solve $u = F_k(T_{k,n})$ for $T_{k,n}$, where F_k is the cumulative distribution function associated with the conditional density function.

Step 3. Construct an ordered pair by drawing a single point from the set $S_1 = \{T_{1,1}, T_{1,2}, T_{1,3}, T_{1,4}\}$ without replacement and a single point from the set $S_2 = \{T_{2,1}, T_{2,2}, T_{2,3}, T_{2,4}\}$ without replacement. The two points, drawn without replacement, constitute a single ordered pair (x_1, x_2). This process is repeated four times, each time drawing without replacement, until all four ordered pairs are formed. Four ordered pairs, so constructed, are illustrated as points in the (X_1, X_2) space below:



Note that the four ordered pairs constitute a sample of size 4 in which each interval associated with X_1 and each interval associated with X_2 is represented.

The values of the dependent variable, Y, associated with each of the sample points in the (X_1, X_2) - space represent four (4) points on the response surface $Y = h(X_1, X_2)$. These four points are illustrated below:



Page 10. The method of constructing random permutations (i.e., permutations of the integers 1,2,3, ..., N each of which has a probability of$(N!)^{-1}$ of occurring) is not made explicit. The authors should, at the very least, give a reference to an algorithm for doing this. A simple algorithm for generating random permutations may be found in a text by Reingold, E.M., Nievergelt, J. and Deo, N., Combinatorial Algorithms, Prentice-Hall, 1977, p.171.

Page 10 (top). The statement, "Furthermore, we randomize so that every combination of cells, eligible under the above restriction, is equally likely to be obtained." is not clear. The question of how the randomization is done is not stated explicitly. Also, the reason why each sample of size N is equally likely is not obvious. Once again, a simple example would suffice. Consider the case in which N=3, and K=2.

Since K=2 the vector $\underset{\sim}{X}$ is two-dimensional; i.e., $\underset{\sim}{X}$ is simply an ordered pair (x_1, x_2). Since N=3 the range space of each of the components, x_1 and x_2, is partioned into three non-overlapping intervals which we shall denote by the integers 1, 2, 3. The notation x_1 (1,2,3) will be used in place of the authors' double subscripted notation $(I_{1,1}, I_{1,2}, I_{1,3})$. When creating a sample of size three, three ordered pairs are formed by combining some permutation of the intervals associated with x_1 with a permutation of the intervals associated with x_2. The specific combinations of x_1 intervals and x_2 intervals from which the actual sample points are drawn are illustrated by the three-by-three checkered patterns shown in the right-hand column of the table presented on the following page. Each of the nine squares in the three-by-three array represents what the authors refer to as a cell.

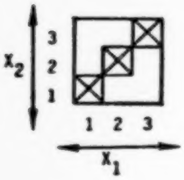
The probability of obtaining a specific permutation of the intervals 1, 2, 3 is 1/3!; hence the probability associated with any pair of permutations is $(1/3!)^2$. There are $(3!)^2$ possible pairs of permutations; however, each sample pattern in the (x_1, x_2)-space corresponds with 3! pairs of permutations. Consider, for example the fifth sample pattern in the following table. The first interval of x_1, is paired with the third interval of x_2. The second interval of x_1 is paired with the first interval of x_2. Finally, the third interval of x_1 is paired with the second interval of x_2. Using the authors' notation we have the following

Permutation of intervals 1, 2, 3 associated with each input variable X_1 and X_2

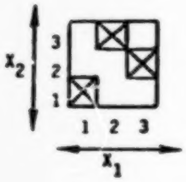
Sample Pattern formed in the (X_1, X_2)-space.

X_1 X_2

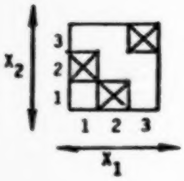
1 2 3 — 1 2 3
1 3 2 — 1 3 2
2 1 3 — 2 1 3
2 3 1 — 2 3 1
3 1 2 — 3 1 2
3 2 1 — 3 2 1



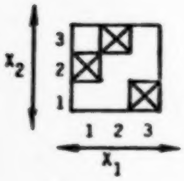
1 2 3 — 1 3 2
1 3 2 — 1 2 3
2 1 3 — 3 1 2
3 1 2 — 2 1 3
2 3 1 — 3 2 1
3 2 1 — 2 3 1



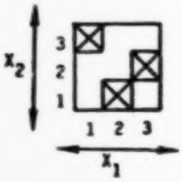
1 2 3 — 2 1 3
2 1 3 — 1 2 3
1 3 2 — 2 3 1
2 3 1 — 1 3 2
3 1 2 — 3 2 1
3 2 1 — 3 1 2



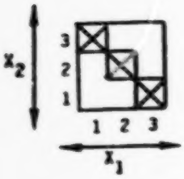
1 2 3 — 2 3 1
3 1 2 — 1 2 3
1 3 2 — 2 1 3
3 2 1 — 1 3 2
2 1 3 — 3 2 1
2 3 1 — 3 1 2



1 2 3 — 3 1 2
1 3 2 — 3 2 1
2 1 3 — 1 3 2
3 2 1 — 2 1 3
3 1 2 — 2 3 1
2 3 1 — 1 2 3



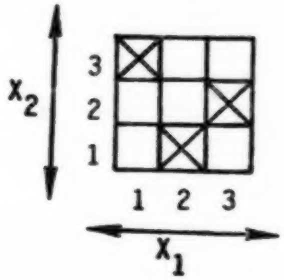
1 2 3 — 3 2 1
3 2 1 — 1 2 3
1 3 2 — 3 1 2
2 1 3 — 2 3 1
3 1 2 — 1 3 2
2 3 1 — 2 1 3



interval pairs: $(I_{1,1}, I_{2,3})$, $(I_{1,2}, I_{2,1})$, and $(I_{1,3}, I_{2,2})$. Each pair of intervals constitutes a cell in the (x_1, x_2)-space. It will be convenient to describe this pairing in the following way

$$\begin{array}{cccc} x_1 & (1, & 2, & 3) \\ & \downarrow & \downarrow & \downarrow \\ x_2 & (3, & 1, & 2) \end{array}$$

The three pairs of intervals (cells) thus formed give rise to the following pattern (of cells) in the (x_1, x_2)-space.



It should be clear that the sample pattern will be invariant under any permutation of the interval pairs. In other words, each of the 3! permutations of the pairs $(I_{1,1}, I_{2,3})$, $(I_{1,2}, I_{2,1})$, $(I_{1,3}, I_{2,2})$ will result in the same pattern of cells in the (x_1, x_2)-space. In terms of the notation used above, the following representations are equivalent, i.e., they each result in the same pattern of cells in the (x_1, x_2)-space:

$$\begin{array}{ccccccccccccccccccc} x_1 & (1, & 2, & 3) & (1, & 3, & 2) & (2, & 1, & 3) & (3, & 2, & 1) & (3, & 1, & 2) & (2, & 3, & 1) \\ & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ x_2 & (3, & 1, & 2) & (3, & 2, & 1) & (1, & 3, & 2) & (2, & 1, & 3) & (2, & 3, & 1) & (1, & 2, & 3) \end{array}$$

Although the above example may be a blinding glimpse of the obvious, it allows one to visualize how the LHS method may be generalized for arbitrary values of N and K.

Since there are N! permutations of the intervals associated with x_1, N! permutations of the intervals associated with x_2, etc., down to N! permutations of intervals associated with x_K, there are $(N!)^K$ ways to combine these intervals. Each combination will describe a specific cell in the K-dimensional space containing the vector $\underset{\sim}{X}$. Note that N! combinations are associated with each sample pattern of cells in the $(x_1, x_2, \ldots, x_K)$-space. Hence, there are $(N!)^{K-1}$ unique sample patterns each having a probability of $1/(N!)^{K-1}$ of occurring.

Pages 11 and 12. The proof of theorem 1 is correct; however, the presentation lacks clarity to say the least. Part of the difficulty stems from the notation and part from the order in which the statements are presented. For example, consider the last sentence on page 11:

> "Since the probability of selecting $\underset{\sim}{X}$ from cell n is $(1/N)^K$, and is the same for all cells, we have
>
> $$E(p_{\underset{\sim}{n}_i} g(Y_i)) = \sum_{\text{all cells } q} E(P_{\underset{\sim}{n}_i} g(Y_i) \mid \underset{\sim}{n}_i \text{ is cell q}) P(\underset{\sim}{n}_i \text{ is cell q})\text{.."}$$

First of all, the mathematical statement which appears above is not a consequence of the word statement which precedes it. Secondly, the mathematical statement should be changed to read as follows:

$$E\left[p_{\underset{\sim}{n}_i} g(Y_i)\right] = \sum_{\text{all } S_{\underset{\sim}{n}_i} \in S} E\left[p_{\underset{\sim}{n}_i} g(Y_i) \mid \underset{\sim}{X} \in S_{\underset{\sim}{n}_i}\right] \cdot P\left[\underset{\sim}{X} \in S_{\underset{\sim}{n}_i}\right]$$

The proof would have been much clearer had the authors proceeded more or less directly as demonstrated below.

By definition,

$$T\left[Y_1, Y_2, \ldots, Y_N\right] = \sum_{i=1}^{N} N^{K-1} \, p_{\underset{\sim}{n}_i} g(Y_i) \quad . \tag{1}$$

Taking the expected value of both sides,

$$E[T] = \sum_{i=1}^{N} N^{K-1}\, E\left[p_{\underset{\sim}{n}_i} g(Y_i)\right] \quad . \tag{2}$$

Since

$$E\left[p_{\underset{\sim}{n}_i} g(Y_i)\right] = \sum_{\text{all } S_{\underset{\sim}{n}_i} \epsilon S} \int_{S_{\underset{\sim}{n}_i}} p_{\underset{\sim}{n}_i}\, g(h(\underset{\sim}{x}))\, \frac{f(\underset{\sim}{x})}{p_{\underset{\sim}{n}_i}}\, d\underset{\sim}{x}$$

and $\quad p_{\underset{\sim}{n}_i} = P\left[x \epsilon S_{\underset{\sim}{n}_i}\right] = \left({}^{1}/_{N}\right)^{K}$

we have

$$E\left[p_{\underset{\sim}{n}_i} g(Y_i)\right] = p_{\underset{\sim}{n}_i} \sum_{\text{all } S_{\underset{\sim}{n}_i} \epsilon S} \int_{S_{\underset{\sim}{n}_i}} g(h(\underset{\sim}{x}))\, \frac{f(\underset{\sim}{x})}{p_{\underset{\sim}{n}_i}}\, d\underset{\sim}{x}$$

$$= (1/N)^{K} \cdot E\left[g(Y)\right] \tag{3}$$

Substituting (3) into (2), yields

$$E[T] = \sum_{i=1}^{N} N^{K-1} \cdot \left({}^{1}/_{N}\right)^{K} E\left[g(Y)\right] = \frac{1}{N} \sum_{i=1}^{N} E\left[g(Y)\right] = \frac{1}{N} \cdot NE\left[g(Y)\right] \quad .$$

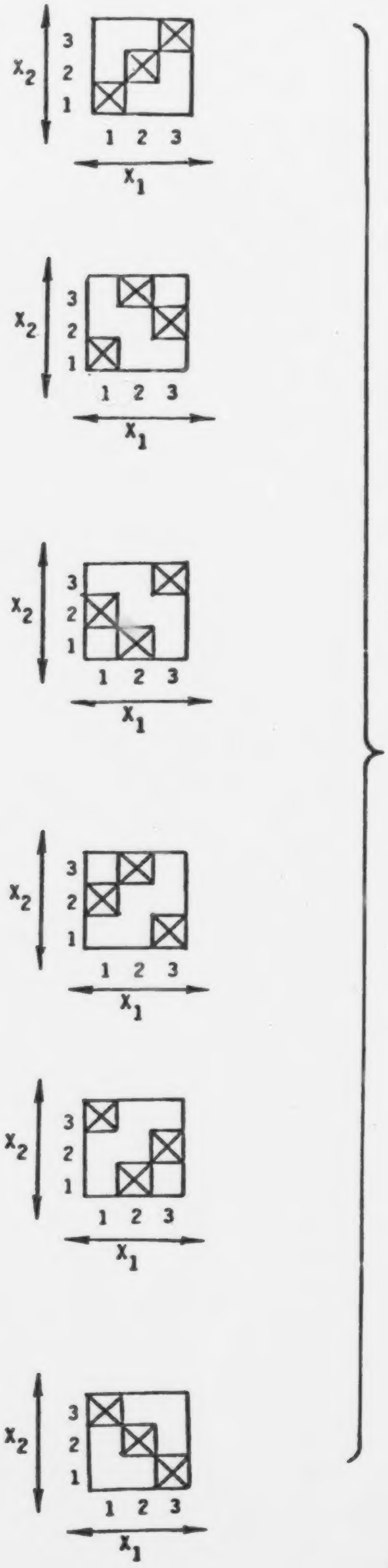
Hence

$$E[T] = E\left[g(Y)\right] \quad .$$

Page 13. The usual nomenclature for the function U(t), defined on page 13 is the unit step function, not the unitary function; cf., Churchill, R., Operational Mathematics, McGraw-Hill, 1958, pp. 5,6.

Page 15 (bottom). The material contained on the bottom of page 15 and on page 16 is relatively clear as is. However, reference to the simple example (N=3, K=2) previously discussed may be helpful. Consider the following diagram:

Six Distinct Sample Patterns in the (X_1, X_2)-space



$(3!)^{2-1}$ distinct cell patterns (see discussion on the top of page D-11).

Page 15. The following statement appears in the first paragraph of Section 2.4:

"In Latin Hypercube Sampling applications the variance of T is usually smaller than the variance of estimators arising from other sampling schemes, but this result may be closely related to the monotonicity property of the code, as we shall see later." This is another example of a vague statement. What do the authors mean by "usually smaller"or "may be closely related"?

The last sentence on page 15 which starts out as follows:

"Let S_{1n_1}, S_{2n_2}, ..., S_{Nn_N}..."

should be changed to read:

"Let $S_{1\underset{\sim}{n}_1}$, $S_{2\underset{\sim}{n}_2}$, ..., $S_{N\underset{\sim}{n}_N}$...".

Page 16 (first paragraph). Note that the ordered N-tuples, denoted by U, correspond to what we have called sample patterns illustrated on the previous page for N=3, K=2. Hence, an alternative argument, based upon the example which appears on page D-13, goes as follows:

In general, there are $(N!)^{K-1}$ distinct cell patterns in the $(x_1, x_2, \ldots, x_K)$-space. Each cell containing an "X" on the previous page represents a cell from which a single sample point (vector) is to be drawn. The three sample vectors $\underset{\sim}{X}_1$, $\underset{\sim}{X}_2$, and $\underset{\sim}{X}_3$ may be assigned to the three cells marked "X" in 3! ways. In general the N sample points (vectors $\underset{\sim}{X}_1, \underset{\sim}{X}_2, \ldots, \underset{\sim}{X}_N$ may be assigned to the $(N!)^{K-1}$ distinct cells in the $(N!)^{K-1} \bullet N!$ ways; hence, the result $(N!)^K$. If the assignment of the labels $\underset{\sim}{X}_1, \underset{\sim}{X}_2, \ldots, \underset{\sim}{X}_N$ to the cells is random, then each of the N-tuples u^i, $i=1, 2, \ldots (N!)^K$ will be equally likely.

Page 16 (6th line from top). Change I_{kn} to $I_{k,n}$.

Page 16 (bottom line). A derivation of Equation 2-29, which reads "var(X) = E [var (X|Y)] + var [E(X|Y)]", should be presented.

Pages 17-31 (General Comments). The examples included in this portion of the report are helpful. They give the reader some insight into the mechanics of the calculations. However, the reasoning behind most of the expressions involving conditional variance is not transparent. The material in this section is, in general, very difficult to understand. It is suggested, once again, that simple examples be used to motivate and illustrate the mathematical results.

Page 21. The authors use the term absolute inequality; the usual expression is strict inequality.

Page 33 (7th line from the bottom). $g(x)/q_n$ should be changed to read $q(x)/q_n$.

Page 33 (3rd line from bottom). This should not be a new paragraph.

Page 33 (last sentence). What are usual circumstances? Also, how small?

Page 34 (3rd line from top). Perhaps, recommendations should be given at the outset relative to the choice of cell sizes.

Page 34 (7th line from top). The term reasonably smooth is not well defined. Certainly a uniform distribution satisfies this condition, but what about other distributions? Of course, the quality of being "reasonably smooth" depends upon the cell sizes as well.

Page 35. The term unitary function which appears on this page should be changed to unit step function (see comment on page D-12 regarding this change).

Page 41. This example is somewhat illuminating. In particular, it is noted that the abscissa in Figure 4.5 is "Total Discharge over 10^6 Years." This quantity is obviously a monotone increasing function of the input variables, a property which is a sufficient condition for the proper use of LHS. One might infer from this that the Sandia work is limited to the calculation of cumulative effects and is of limited value in studying, for example, the dose to an individual at some future time.

Pages 41-49. The reference site described on pages 41-49 as used throughout the series of Sandia reports, e.g., NUREG/CR-1377. It would be advisable for the authors to use the same list of variables for the characterization of radionuclide transport phenomena. In particular, seven variables are listed on page 47. Two of these, namely the distribution coefficient of the isotope and the leach time, have been identified as important variables. Actually, some functions of these variables have been identified as important variables on page 52 of this report. Ten independent variables (input variables) have been listed on page 31 of NUREG/CR-1377. It is not clear how the two lists are related, if at all. This may be considered a minor point; however, we recommend that the set of input variables, the assumptions and the conclusions relative to this example be consistent throughout the series of reports in which this example appears.

Page 47. No consideration has been given to radioactive decay of the repository material. Furthermore, it is assumed that ground water begins leaching the waste immediately. Therefore, the results should not be interpreted as indicative of a waste repository performance.

Page 50 (second paragraph). The authors make the following statement:

> "The computer program's output variable Y for this example is the total discharge of an isotope in the 10^6 years following burial of the radioactive waste."

The unit associated with total discharge of an isotope is not specified. Is total discharge measured in liters, cubic meters, grams, curies, or some other unit? The same comment applies to the labels associated with the abscissae of all the figures which follow this discussion, i.e., Figures 4.5-4.16.

Page 51. (Figure 4.5) The ordinate scale is not labeled correctly. The ordinate is not the "estimated distribution function". It should be labeled Pr[Total Discharge $<$ D], where D denotes the values listed along the abscissa.

The same comment pertains to Figures 4.6 (page 64), 4.7 (page 65), 4.8 (page 66), 4.9 (page 69), 4.10 (page 70), 4.11 (page 71), 4.12 (page 72), 4.13 (page 73), 4.14 (page 74), 4.15 (page 75), 4.16 (page 76), and 5.5 (page 111).

Page 52. (Section 4.3) Reference should be made to the actual analysis in which the variables X_4 and X_5 were identified as important variables. The reader should be allowed to examine the analysis and see exactly how the ranks were determined. The large values which appear in Table 4.1 may result in the reader's questioning the real importance of X_4 and X_5.

The last sentence on page 52 reads as follows:

> "In order to aid the reader in pairing individual observations with the new weights given in the next section we provide in Table 4.1 a complete listing of the Latin hypercube sample for both X_4 and X_5 as well as the rank of the specific observation and the interval from which the observation was selected."

This is all that is said about Table 4.1. Persumably, this statement expresses the author's motivation behind Table 4.1. It is certainly not clear what the reader is expected to do with the data in Table 4.1, if anything. The reader is left wondering what he or she is supposed to observe in Table 4.1. As a matter of fact, Table 4.1 generates more questions than it answers. The same comments also apply to Table 4.2; however, a little more is said about the entries in Table 4.2 than was said about Table 4.1.

Page 63. (Second paragraph) It is not clear that the results contained in Table 4.2 are illustrated in Figures 4.6 - 4.8. Figures 4.6 through 4.8 show how the estimated distribution functions of total discharge over 10^6 years compare with the so called base case under the three assumptions regarding the distributions of X_4 and X_5. The weights themselves are not illustrated in any way; hence, the statement contained in the second paragraph on page 63 is meaningless.

Page 63. (Bottom) The following statement appears on the bottom of page 63:

> "The estimate S'(y) appears to be a reasonable estimate of the true distribution function, but it is not possible to tell from this one example whether the size of the differences beteeen S(y) and the "true" c.d.f. is what we might expect due to sampling fluctuation."

Unless some means of testing the goodness of fit of an empirical c.d.f. obtained via the LHS method is developed, no one will ever be able to make any statements, other than subjective statements, regarding how well the LHS method works with respect to the empirical distribution functions so derived.

As a matter of fact, questions regarding the limitations imposed by the LHS method, specifically, the inability to apply the usual goodness of fit tests such as the chi-squared test or the Kolmogorov-Smirnov test, should be examined in depth.

Pages 64-66. (Figures 4.6-4.8) Figures 4.6 through 4.8 contain a representation of what the authors call the "true" c.d.f.

It should be pointed out that there is no more truth to these c.d.f.'s than any of the others. Presumably, a confidence interval on the "true" c.d.f. will be narrower than a confidence interval associated with the other c.d.f.'s due to the larger sample size associated with the so called "true" c.d.f.

A much more convincing demonstration of the LHS method would involve a problem in which the actual c.d.f. of the output variable is known a priori. Several possibilities come to mind immediately. Why not apply the LHS method to an example involving a linear combination of Gaussian distributed (input) variables, say $Y = \alpha_1 x_1 + \alpha_2 x_2 + \dots + \alpha_K x_K$. Alternatively, the distribution of $Y = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_K^{\alpha_K}$ will be lognormal provided the x_j's are stochastically independent lognormally distributed random variables. Each of these cases take advantage of the fact that certain distributions are self-replicating under certain algebraic operations. Other distributions for which this is true include the gamma distribution which exhibits a mean conserving property under addition and the beta distribution which is self-replicating under multiplication provided certain conditions are met.

Page 77 Section 4.6. The comparison of LHS, replicated LHS, and random sampling was informative. However, in the examples shown, it does not seem that very much has been gained by the effort that has gone into LHS compared to random sampling. The standard deviation associated with LHS estimates is smaller than that of random sampling (Figure 4.18); however, the results of waste repository calculations are uncertain by at least a factor of 10, so the refinement of LHS seems a bit futile.

Page 88. (Second paragraph) The following statement appears:

> "The number of runs (i.e., the sample size) should be large enough to provide good separation or grouping of scenarios, and yet should be within the inherent time and cost constraints."

We agree with this statement; however, sample size has no impact on the "separation" of scenarios, whatever that means. Separation implies distance between. I believe the authors really mean that as the sample size increases, smaller and smaller differences between output variables may be detected.

Page 91. (Table 5.1) Fourteen input variables are listed in Table 5.1. How do these relate, if al all, to the fourteen variables listed in Table 2 on page 31 of NUREG/CR-1377? Since the reference site is the same in both reports it seems reasonable to expect a certain amount of consistency among the variables that are used to characterize radionuclide transport at this reference site (c.f. the comment on page D-16 relative to pages 41-49).

Page 110 Para. 1. "In fact, a scenario which has no discharge (one which we haven't considered in this paper) would most likely have a much larger probability associated with it than all other scenarios combined. However, these simplifying assumptions will not affect the general application of the procedure."

The question of completeness is hardly a simplifying assumption and the neglect could lead to erroneous results. The Sandia work seems to give little or no consideration to scenarios and geologic changes which prevent release.

Page 113 Para. 2. The requirement of monotonicity is again stated without any discussion of the limitation it imposes on the method.

Page 114 Para. 2. The conclusion of sample sizes of 100 to 200 was found in a fairly special case for a limited number of variables. If the number of variables approaches several hundred, as stated earlier in the report, it seems clear that the sample size number would need to be larger.

For scenario testing, it is not clear that the LHS method is needed, let alone sample sizes of 4 or 5. The scenarios could be run on the basis of the mean values of the variables.

APPENDIX E

DOCUMENT 5

"Scenario Development and Evaluation Related to the Risk Assessment of High Level Radioactive Waste Repositories"

Page 1,2. This is a good introduction to the transport problem. However, "convection" implies movement of fluid due to uneven temperatures. Since we are only considering an isothermal system, "convection" does not appear to be appropriate. Another term should be used, e.g., groundwater flow; otherwise further explanation is required.

Page 2 Para. 3. Heat strongly affects chemical processes and the water pH affects the ion-exchange retardation. Neither of these are mentioned.

Page 2 Para. 4. Nuclide decay results in a change of chemical species from mother to daughter. The ion-exchange migration retardation changes with this change of species.

Page 3 Equation 1.1.

$$\partial/\partial x_{\alpha}(D_{\alpha\tau}\partial C_i/\partial x_{\tau}) - \partial/\partial x_{\alpha}(C_i V_{\alpha}) + \sum_{j+1}^{n} R_{ij} = \partial(\epsilon C_i)/\partial t$$

$$\alpha, \tau = 1,2$$

The authors say that the dispersion-convection equation, displayed above, accounts for all significant chemical and biological processes. This is not completely correct in that it does not account for health effects.

Other limitations of the equation should be discussed. R_{ij} is a source term for isotope j decaying to isotope i. There should also be a term for i decaying to something else, say m, which is missing. R_{ij} is a spatially dependent large source resulting from these migrations and decays; this spatial dependence is not indicated. There should be an R_{ij} source that is spatially confined due to the decay from j to i at the place of burial and an R_{ii} term which represents those nuclides buried as species i and leached as species i. R_{ij} should also be time dependent to represent the leaching of nuclear wastes.

Page 3 Para. 6. I don't know what the authors mean by, "one for each of the contaminants and one for each of the major or minor ions that could interact with the radioactive species."

Page 4 Para. 1. "Such an assumption seems justifiable for at least two reasons. First, a suitable model of anisotropic dispersion does not exist; second, evidence suggests that the practice of assigning large microscopic dispersivity values for many kinds of porous media might not be adequate for describing transport in certain media (6)."

The second reason does not seem to explain the reason for the longitudinal and transverse dispersion coefficients.

Page 4 Para. 4. Why do the authors write about a three-dimensional anisotropic tensor when they just explained they are only working in two dimensions and assuming isotropy?

Page 4 Para. 4. "The simulations undertaken in this work are based on the transport of a so-called "perfect tracer" that neither decays radioactively nor interacts with the porous medium." This seems to say that R_{ij} is only R_i, probably a function in space and is not retarded through ion-exchange. This reduces the problem to just a flow-field problem, and hence a solution of Darcy's equation. In Appendices A and B a cation exchange capacity term is listed; hence, the authors appear to apply ion-exchange retardation by strata, not by chemical species.

Pages 3, 4 & 5. Terms should be defined immediately after Equations 1.1, 1.2, and 1.3.

Pages 4 & 5. The assumptions of a "perfect tracer", that neither decays radioactively nor interacts with the porous medium, and an "isothermal system in granite" are very conservative. This conservatism should be emphasized here.

Page 7 Para. 7. Why is DCPT inherently stable and immune to cumulative numerical dispersion? It would seem that, given the solution of the flow field, the addition of dispersion would lead to inherently stable results.

Page 8 Para. 1. Where is the radioactive waste located in the host rock? Is it a point source, line source or an area source? How much salt must be penetrated before the waste gets to other zones?

Page 8 Table 2.1. While these parameters appear to be consistent with Campbell et. al., NUREG/CR-0458, they appear to be quite conservative. It seems that a data evaluation activity is needed to arrive at realistic parameters for use in repository evaluation models.

Page 8. The treatment of salt as a porous medium is questionable. While some salt mines may be "wet", perhaps due to an inadequate shaft seal, and salt beds may be removed by circulating groundwater a different scenario from the one being considered here, there is no clear evidence that groundwater moves through rock salt, especially in any salt bed that would be used for a repository.

Page 9 Para. 1. What is the basis for 5 feet and 0.25 feet horizontal and longitudinal dispersivity, respectively?

Page 9 Para. 3. Is it realistic to have all sides except the top as no flow boundaries?

Page 9. Although the boundary conditions are not unreasonable, they only represent one set of physically realizeable boundary conditions. Other boundary conditions might yield vastly different results.

Page 10 and Appendix B. The hydraulic conductivity of granite used is overly conservative. Based on Swedish work, a more realistic range of hydraulic conductivities would be 10^{-4} to 10^{-6} ft./day (rather than the $10^{-0.89}$ to $10^{-2.59}$ ft./day used in this study).

Page 10 Para. 2. It is commendable that the authors have listed the input and output data to assist others in reproducing their results.

Page 11. Why didn't the authors take as a reference site the one used and extensively studied by the Swedes (KBS Volume I, "Handling and Final Storage of Unprocessed Spent Nuclear Fuel")?

Page 11 Para. 3. How would a user gauge or estimate the loss of accuracy due to the time steps being used?

Page 13. The concentration values are neither defined nor are the units specified. This is true of the text and the figures.

Page 14 Figure 2.1 (upper). Usually it is assumed that the volume containing the radioactive wastes is a small fraction of the volume of the salt zone; i.e., one generally assumes that a considerable flow distance through salt is required to reach the waste. Also, one generally assumes that a considerable flow distance is necessary to exit the salt. This figure indicates that the repository takes up the whole salt (disposal) region.

Pages 14 & 15. The numbers of the geologic units should be added to the geology cross-sections.

Page 16. Head distribution should be defined and the units stated.

Page 16 Figure 2.3 (upper and middle). Since it is assumed that a fault goes through the repository at grid locations 23 and 24, why doesn't this show up in the conductivity data?

Page 16 Figure 2.3 (lower). The authors do not state how the steady state head distribution is calculated. From Figure 2.1 upper, it is apparent that the head drops from 6000 feet in the upper left hand corner to 1000 in the lower right hand corner; however, Figure 2.3 (lower) shows no evidence of this head. In fact, the constant gradient lines generally tend to be vertical. Since the flow is perpendicular to the head gradient, the net effect would be a longitudinal flow, not in the direction of the gravitational gradient. Clearly, this requires further explanation.

Page 17 Figure 2.4. What are the units of concentration? What is the meaning of the percentage? Presumably, the effect is due to the fault since it occurs at that location. The authors should show what would be the effect if the fault were not there; especially since the conductivity was not changed in the fault zone.

Page 17. Why change the vertical scale? Why not make the vertical scale 1 cm/600 feet throughout? It would allow the grid and the hydraulic head distribution to be superimposed on the distribution of concentration diagrams.

Page 19 Para. 3. Why was 3 orders of magnitude chosen for the disruptive zone?

Page 20. Add vertical lines to table heading for greater clarity.

Page 21 Para. 1. Why did the disruptive zone only penetrate units 2, 3 and 4? It would seem that salt would be the least likely to fault due to its ductility.

Page 21 Para. 3. Apparently the explanation for Figure 2.3 is contained on this page; i.e., the fault shown in Figure 2.1 is assumed not to exist. Nevertheless, what are the units of concentration? Does the percentage refer to the total amount of the salt zone removed? How was 36,000 years obtained? The plots are 4×10^4, 12×10^4, and 20×10^4 years.

Page 22 Para. 1. How can one tell that the groundwater flow pattern is not significantly changed?

Page 22. How realistic is a low conductivity disruptive zone?

Page 25 Para. 3. The negative log ratios seem to indicate that the confinement times have been increased for this case relative to the reference case. This contradicts what has been stated.

Page 26 & 27. Units 5 and 6 are not properly defined. The discussion is confusing. The justification for the last concluding statement on page 27 is not clear.

Page 27 Para. 1. It is not obvious that further reduction of hydraulic conductivity will yield the stated effect. Figure 3.32 (top) and Figure 3.7 look identical. Figure 3.32 (middle) shows contours of -0.5 and a contour of 0.5, but so does Figure 3.32 (top). Figure 3.32 (bottom) shows a contour of 1.0 but contours this high appear in the other figures. Therefore, it does not seem that the conclusions are demonstrated.

Page 28 Figure 3.1. Why doesn't the hydraulic head show the effects of the fracture zone?

Page 29 Figure 3.2. What is the meaning of the logarithm of exit time ratios? Is it a base 10 logarithm? Perhaps it would be clearer, for the average reader, if the authors had given the ratios.

Page 30 etc. Repository locations should be marked by symbols. Numbers representing concentrations are confusing; only the percentage number appears to have any meaning.

Page 34. The meaning of Figure 3.7 is not clear.

Page 61, 62. Residence times are extremely short. Such short times might apply to very fractured and/or weathered granites. They are not realistic for competent, carefully selected granite masses at depths of 2,000 feet or more.

Appendix B Table B.1. What is the meaning of a CEC value of 5? Does this mean that the isotope migrates faster than the water flow?

Appendices A and B, Tables A.4 and B.4. Why don't the head values in the tables bear any resemblance to the steady state head distributions shown in Figures 2.3 and 3.33? Why does the head increase from right to left although the repository is not tilted? Why does the head increase with depth?

[redacted]

GLOSSARY OF ACRONYMS

DPCT - Deterministic-Probabilistic Contaminant Transport - a method for calculating groundwater radionuclide transport using the flow field as the primary determinant with a Guassian distribution accounting for the probabilistic dispersion.

DVM - Distributed Velocity Method - a method of calculating groundwater radionuclide transport based on the distribution of flow velocities from source to sink. This is essentially a Green's Function method using superposition.

LHS - Latin Hypercube Sampling - a stratified sampling procedure which ensures that the full range of each variable is represented by each sample point.

NWFT - Network Flow and Transport - a one-dimensional code for calculating groundwater radionuclide transport.

SWIFT - Sandia Waste Isolation Flow and Transport - a three-dimensional finite difference code for calculating groundwater radionuclide transport.

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This project is an independent review of products from a NRC research program to develop a risk-based methodology for assessing the long-term risk of a nuclear waste repository in a geologic medium. This report presents a review of five technical reports. Two of the documents concern with geosphere simulation and three of the documents pertain to statistical methods including the application of Latin Hypercube Sampling.

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